2018 SUMMER

UNDERGRADUATE RESEARCH SYMPOSIUM

WEDNESDAY, JULY 25

9:30am - 11:45am

Jordan Hall of Science Galleria

ROSTER OF STUDENT RESEARCHERS

#	STUDENT RESEARCHER	PROJECT TITLE	ADVISOR	DEPARTMENT
69	**Angela Abarca Perez**	Investigation of the sorption behavior of organic acids onto catalytic- and food-grade titanium dioxide nanoparticles	Dr. Kyle Doudrick	Civil and Environmental Engineering and Earth Sciences
24	**Hunter Allen**	VASP Calculations and Reactor Design for Ethylene Oligomerization	Dr. Jason Hicks, Dr. William Schneider	Chemical and Biomolecular Engineering
47	**Maria Amenabar Farias**	Stay the Course™ Improves Community College Persistence and Completion	Dr. James Sullivan	Economics
1	**Apple J. Amos**	Lab on a Chip: Early Cancer Detection Using Anion Exchange Membranes in Microfluidic Devices	Dr. Satyajyoti Senapati	Chemical and Biomolecular Engineering
61	**Gabriela Aquino**	"Use Your Words": The Role of Emotional Security on Interparental Conflict	Dr. E. Mark Cummings	Psychology
2	**Bowen Ashenfelter**	Mapping of Lead Levels within the South Bend Community	Dr. Marya Lieberman	Chemistry and Biochemistry
66	**Corey Atwell**	Influence of Annealing on the Controlled Growth of CsPbBr3 Nanocrystals	Dr. Prashant V. Kamat	Chemical and Biomolecular Engineering
23	**Jonathan Austin, Breanna Belz, Angel Rodriguez**	Feasibility of Vehicle-Wake Energy Extraction by Roadside Wind Turbines	Dr. Eric Matlis	Aerospace and Mechanical Engineering
7	**Kyle Barrentine**	Can personality influence how you manage a social network?	Dr. David Hachen	Sociology
35	**Stephen Bauer, Mark Etzelmueller**	Development of Microimplants for Deep Tissue Optical Sensing	Dr. Thomas O'Sullivan	Electrical Engineering
25	**Tyler Bear**	Synthesis and characterization of iptycene-based polyimides with tunable chain rigidity for gas separation membranes	Dr. Ruilan Guo	Chemical and Biomolecular Engineering
48	**Kendrea Beers**	Exhaustive Heterogeneous Graphlet Counting for Network Alignment	Dr. Tijana Milenkovic	Computer Science and Engineering
44	**Margaret Bielski**	An Analysis of Lead in Local Roads, Homes and Historical Industries: How South Bend's History is Poisoning its Children	Dr. Marya Lieberman	Chemistry and Biochemistry
8	**Abigail Boatwright**	An Analysis of Intellectual Property Diffusion in Global Markets	Dr. Paul Brenner	Economics
26	**Gabriel Brown**	Development and Characterization of Plasma Catalytic Reactors	Dr. David B. Go	Aerospace and Mechanical Engineering
67	**David Brown**	Designing Energy Efficient Diafiltration Units around Membranes that Separate Molecules of Comparable Size	Dr. William Phillip	Chemical and Biomolecular Engineering
70	**Mariana Calderon**	Casting polyvinylidene fluoride (PVDF) using the vapor-induced phase separation (VIPS) method	Dr. William Phillip	Chemical and Biomolecular Engineering

32	**Santiago Calderon Novoa**	Synthesis and performance testing of pentiptycene-based polymeric membranes for mixed gas separation	Dr. Ruilan Guo	Chemical and Biomolecular Engineering
49	**Kevin Choy**	A Web-Based Tool for Flexible Learning-Free Segmentation And Reconstruction for Sparse Neuronal Circuit Tracing	Dr. Walter Scheirer	Computer Science and Engineering
9	**Carl Colglazier**	Advancing the Tools for Global-Scale Computational Social Science.	Dr. Paul Brenner	Computer Science and Engineering
65	**Quentin Colo**	Comprehensive Case Management to Lift Families Out of Poverty	Dr. James Sullivan	Economics
36	**Emma Conroy, Nicole Nemeth**	Extra-pair Parentage in Field Sparrows (Spizella pusilla)	Dr. Joel Ralston	Biology
62	**Daniel Copeland**	Landscape Effects on the Gut Community of Long-Tailed Macaques	Dr. Hope Hollocher	Biological Sciences
40	**Chloe Crusan**	RadioHound: A low cost spectrum sensor	Dr. Bertrand Hochwald	Electrical Engineering
78	**Gabriel Cruz-Ruiz**	New nanocapsules for drug delivery	Dr. Bradley Smith	Chemistry and Biochemistry
27	**Anthony Deziel**	Synthesis and Characterization of Platinum (II) Carbene Complexes	Dr. Vlad Iluc	Chemistry and Biochemistry
45	**Michael Dowd**	Development of a Paper-Based Colorimetric Test to Detect Oxytocin	Dr. Marya Lieberman	Chemistry and Biochemistry
58	**Alison Doxey**	Long-Run Effects of College Openings: Evidence from U.S. Historical Data	Dr. Kasey Buckles	Economics
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59	**Bailee Egan**	Investigating Patterns of the Gut Microbiome in Long-Tailed Macaques	Dr. Hope Hollocher	Biological Sciences
37	**Maria Escobedo**	Modeling Equilibrium Reactions with Origin	Dr. Kristin Kuter	Mathematics and Computer Science
51	**Diego Fernández**	Lobster: Harnessing Opportunistic Clusters with a Workflow Management Tool for CMS Data Analysis	Dr. Kevin Lannon	Physics
10	**Anne Freeman**	Developing Software to Process Malaria Genetic Data for QTL Analysis in a Shared Parent Genetic Cross	Dr. Michael Ferdig	Biological Sciences
34	**Jacob Galden, Paula Murphy**	Stretchable Polymer Composite Film with Extreme Ductility and Toughness	Dr. Tengfei Luo	Aerospace and Mechanical Engineering
52	**Jon Genty**	Classifying Aging- and Non-Aging-Related Genes in Dynamic Protein-Protein Interaction (PPI) Networks	Dr. Tijana Milenkovic	Computer Science and Engineering
11	**Jacob Gersfeld**	SNP Isolation and Primer Design in R. pomonella	Dr. Jeffrey Feder	Biological Sciences
53	**Nicholas Grasley**	Using Crowd-Sourced Genealogy to Analyze the Long-Run Effects of Prohibition	Dr. Kasey Buckles	Economics

12	**Eric Gronda**	Visual Analytics of Student Clickstream Data Using Higher Order Networks	Dr. Chaoli Wang	Computer Science and Engineering
71	**Nishtha Gupta**	Elucidating fundamental processing property relationships for chemically patterned membranes	Dr. William Phillip	Chemical and Biomolecular Engineering
3	**Citlali Gutierrez**	From the Field: Development of a Reliable and Affordable Home Lead Test Kit	Dr. Heidi Beidinger	Biological Sciences
82	**Loren Hahn**	Turbomachinery Sensing: Analysis and Optimization	Dr. Thomas Pratt	Electrical Engineering
39	**Hannah Himes**	Quantifying the Relationship between the Gut Microbiome and Blastocystis in Long-tailed Macaques	Dr. Hope Hollocher	Biological Sciences
63	**Aurora Hurtado Olivas**	Probing the Mechanism of Osmium Mediated Carbon-Sulfur Bond Cleavage Using Unsymmetrically Substituted Ligand	Dr. Seth N. Brown	Chemistry and Biochemistry
13	**Allie Johnston**	Are all Personality Inventories Equal? Assessing the Applicability of the BFI-2 to Adolescents	Dr. Ying (Alison) Cheng	Psychological and Educational Measurement Lab
60	**Elisabeth Kerns**	Perovskite Characterization and Degradation	Dr. Prashant V. Kamat	Chemistry and Biochemistry
14	**Khaya Klanot**	Deep Learning for Particle Physics: Investigating Neural Network Structure and Hyperparameters	Dr. Kevin Lannon	Physics
68	**Anna Kluender**	Understanding Lower Critical Solution Temperature Ionic Liquids in the Development of Revolutionary Absorptive Cooling Fluids	Dr. Brandon Ashfeld	Chemistry and Biochemistry
38	**Kerrie Koller, Kailey Novack**	Creating a Catalog for Albendazole Paper Analytical Devices	Dr. Ian Bentley	Chemistry, Physics
83	**Henadz Krukovich**	Tracking multiple targets using Dual-Polarized Antennas with Software Defined Radios	Dr. Thomas Pratt	Electrical Engineering
41	**Tristen Lewandowski**	Programmable and Reconfigurable Millimeter-Wave Circuits and Antennas	Dr. Jonathan Chisum	Electrical Engineering
75	**Laurel Anne Lown, Mary Green**	Validation of the MicroBio PAD by testing drinking water quality in Nepal	Dr. Don Paetkau	Biology
19	**Lizbeth Lucero**	Infant and Child Mortality Rates and the Role of Female Education: A Meta-Analysis of Statistically Significant and Insignificant Research	Dr. Erin McDonnell	Sociology
84	**Marina Malone**	Integrated Task and Motion Planning for Robotic Systems	Dr. Hai Lin	Electrical Engineering
28	**Ana Martinez**	Coordination Chemistry of the Human Copper Transporter	Dr. Kathryn Haas	Chemistry
54	**Rachel McCarthy**	Predicting Body Image through Self-Esteem and Social Networks	Dr. David Hachen	Sociology
29	**Madison Mettey**	Synthesis of transition metal alumosiloxide complexes as models of zeolite active sites for energy-related catalysis	Dr. Emily Tsui	Chemistry and Biochemistry
76	**Heather Miller**	The Development of a Yeast Biosensor for the Detection of Prednisone	Dr. Don Paetkau	Biology

20	**Christopher Monjaras**	The Effects of Mandatory Retirement on Employee Health Outcomes	Dr. William Evans	Economics
64	**Eduardo Morales-Rivera**	Comparison of Two Dual Spring-Loaded Inverted Pendulum Models of Sloped Walking	Dr. James Schmiedeler	Aerospace and Mechanical Engineering
33	**Brizzia Munoz Robles**	Targeting therapeutics through supramolecular affinity	Dr. Matthew Webber	Chemical and Biomolecular Engineering
30	**Lee Ngochi**	Synthesis of Nickel Phosphide on Aluminum Oxide	Dr. Jason Hicks, Dr. William Schneider	Chemical and Biomolecular Engineering
72	**Erin O'Brien**	Improving Drug Efficacy Through Supramolecular Affinity	Dr. Matthew Webber	Chemical and Biomolecular Engineering
4	**Samantha O'Connor**	Optimization of antimicrobial activity of truncated linear variants of enterocin AS-48	Dr. Shaun Lee	Biological Sciences
79	**Olanrewaju Olafuyi**	Computation Spectroscopic Analysis of Alpha Amyloids of PSMα3	Dr. Arnaldo Serrano	Chemistry and Biochemistry
15	**Luke Onken**	Utilizing a Bayesian Point Process Model to Predict Forest Fires from Charcoal Data	Dr. Jason McLachlan	Biological Sciences
80	**Robert Ornelaz**	Does Cultural Conflict Affect educational Attainment?	Dr. Rory McVeigh	Sociology
5	**Andrew Pendergast**	A low-cost 3D-printed electrophoretic method for proteomics sample preparation	Dr. Matthew Champion	Chemistry and Biochemistry
81	**Carolina Ponce**	Reproductive Health Fears Present in Nahua Indigenous Women: An Analysis of Interactions with Biomedical Personnel	Dr. Vania Smith-Oka	Anthropology
21	**Allen Porterie**	Performing Black Masculinity	Dr. Mark Sanders	English
55	**Nicholas Potteiger**	Archiving Workflows Onto Cloud Based Storage	Dr. Douglas Thain	Computer Science and Engineering
16	**Kang Pu**	Knowledge Diffusion in the Global Automotive Industry	Dr. Paul Brenner	Computer Science and Engineering
73	**Rebecca Radomsky**	Design of Experimentation to Test Faradaic Efficiencies of Plasma-Liquid Systems	Dr. David B. Go	Chemistry and Biochemistry
22	**Victor M. Rey Davila**	Light Activated Synthesis of Au Nanoplates	Dr. Svetlana Neretina	Aerospace and Mechanical Engineering
85	**Daniel Riehm**	Using Augmented Reality to Control a Six-Axis Robot Arm	Dr. Richard Billo	Electrical Engineering
31	**Aaron Roe**	Computational Identification of Anharmonic Vibrational Frequencies for Brønsted Acid Sites in Aluminum Substituted Chabazite	Dr. William Schneider	Chemical and Biomolecular Engineering
86	**Robert Schenck**	Wireless Communications Interface and Services for Drone Swarms	Dr. J Nicholas Laneman	Electrical Engineering
42	**Adrian Siwy**	Optically-Controlled Tunable Microwave and Millimeter-Wave Devices for Adaptive Wireless Communications	Dr. Lei Liu	Electrical Engineering

77	**Erica Slogar**	Copper(I) & Copper(II) binding to the ectodomain of human Ctr1	Dr. Kathryn Haas	Chemistry, Physics
6	**Kyle Smith**	Phosphate Detection Using Yeast Produced CO2	Dr. Holly Goodson	Chemistry and Biochemistry
56	**Jeremy Speth**	Generation and Matching of Bipartite Graphs	Dr. Peter Kogge	Computer Science and Engineering
43	**Spencer Spitz**	Passive, Crowd-Sourced WiFi Characterization	Dr. Aaron Striegel	Computer Science and Engineering
46	**Maxwell G. Tetrick**	Getting High on Science: Surface-Enhanced Raman Spectroscopy for Illicit Drug Detection	Dr. Jon P. Camden	Chemistry and Biochemistry
74	**Margo Waters**	Magneto-Electric Silica Nanoparticles (Mag-E-Si-Ns) for Combinatorial Chemotherapeutics Against Metastatic Cancers	Dr. Prakash Nallathamby, Dr. Paul Helquist	Aerospace and Mechanical Engineering, Chemistry and Biochemistry
87	**Jeremiah Yohannan**	Human-Robot Collaboration	Dr. Hai Lin	Electrical Engineering
17	**Qimin Zhang**	Reduction of Resources Consumption in Parallel Applications Using a Density-based Clustering Model	Dr. Douglas Thain	Computer Science and Engineering
57	**Yuekai Zhang**	Knowledge Diffusion in Global Commerce, Investment and Research	Dr. Paul Brenner	Computer Science and Engineering

POSTER SESSION 1: 9:30 – 10:30 A.M.

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Lab on a Chip: Early Cancer Detection Using Anion Exchange Membranes in Microfluidic Devices

Apple J. Amos
Chemical and Biomolecular Engineering
College of Engineering

Faculty Advisor: Dr. Satyajyoti Senapati
Grad Student or Postdoctoral Mentor: Zeinab Ramshani

Breast cancer is the most common cause of cancer among women with approximately 1.7 million new cases annually and nearly 0.5 million deaths worldwide per year. As with most diseases and chronic illness, its treatment is more effective in its early stage. Hence, the early detection of the breast cancer receptors (ER, PR, and HER2) can significantly reduce the cancer mortality rate. Towards this direction, I am working on a project to develop a rapid, sensitive and selective protein detection platform using an ion-exchange membrane (IEM)-based sensing technology that has been successfully used to detect different nucleic acid cancer biomarkers. My project is aimed to detect breast cancer HER2 biomarker using an ELISA sandwich assay scheme where a DNA conjugated reporter antibody is used to register a change in the current-voltage signal on successful docking of the target biomarker with the detection antibody attached on the membrane surface. The detection selectivity is achieved by using the shear flow to remove the non-specifically bound non-targets from the sensor surface. I have able to attach and detect proteins using the IEM sensor, but the results are not very repeatable. These results indicate the original goal of this project is possible though not conclusively proven to work and requires more testing.

Mapping of Lead Levels within the South Bend Community

Bowen Ashenfelter
Chemistry and Biochemistry
College of Science

Faculty Advisor: Dr. Marya Lieberman
Grad Student or Postdoctoral Mentor: Meghanne Tighe
Other Contributors: Mark Wilson, George Ruscio-Atkinson

Lead poisoning is a universally understood concept, but many people in South Bend are not aware of the danger that lead poses to their families. Lead poisoning isn't much of a concern for adults, but for children it can be a silent, health hazard. Our lead team has spent the last few weeks collecting soil and paint samples from the Near Northwest Neighborhood (NNN) to test the lead concentrations. We traveled down roadsides and alleys collecting and GPS tagging both soil and paint chips (n=320) from every property within the NNN. An X-Ray Fluorimeter (XRF) was used to determine the concentration of the lead in the soil and paint chips. This allowed for the lead levels to be mapped and analyzed using geographical information systems.

The EPA guidelines suggest that children should not play in areas where the soil has a lead level of 400 ppm, and such soil should not be used for gardening. We found many sites where the lead level in the soil was at or above this level. Our map of soil lead levels will help South Bend residents understand their exposure risk from lead in the soil. As part of the greater ND LIT initiative, we are working to provide the community with information to help spread awareness and manageable methods to reduce the exposure to lead hazards.

From the Field: Development of a Reliable and Affordable Home Lead Test Kit

Citlali Gutierrez
Biological Sciences
College of Science

Faculty Advisor: Dr. Heidi Beidinger
Grad Student or Postdoctoral Mentor: Katlyn Sawyer
Other Contributors: Michael Dowd, University of Hawaii at Manoa;
Margaret Bielski, Chris Knaub, Marya Lieberman, Claire Marks, Michelle Ngai, Lane Nicolay, Graham Peaslee, Matthew Sisk, Meghanne Tighe, University of Notre Dame;
and Danielle Forbes, University of Toledo

Background: The legacy of leaded paint and gasoline continues to pose health risks for children in our community. St. Joseph County's Census Tract 6 has one of the highest rates of elevated blood lead levels in Indiana. Creating a reliable, consumer friendly home lead test kit that detects lead hazards within homes can help families prevent elevated blood lead levels in their children. The goal of this lead test kit is to reverse the current paradigm of using children as beacons to detect lead in their home environment. The kit allows families to collect three dust samples, three soil samples, and two paint chips.

Methods: Two teams were established: (a) field team and (b) lab team. Engaging the principles of Community-Based Participatory Research, CBPR, the field team collaborated with community partners to recruit 50 participants in St. Joseph County to test the kit in their home. The field team conducted two home visits for each participant. Visit One served to obtain consent, complete a questionnaire, and build rapport. Visit Two served to observe participants' use of the test kit and to conduct on-site X-Ray Fluorometer, XRF, analyses. Two individuals from the lab team analyzed kit samples with an XRF. Lab and field results were blinded.

Results: The number of homes tested was 26. Two homes were thrown out of the study due to data collection error. Of the 24 homes, 9 were built pre-1950, 7 homes were built between 1950-1978, and 8 homes were built after 1978. All pre-1950 homes had at least one sample at or above EPA actionable level. Meanwhile, 42.9% of homes from 1950-1978 had at least one sample at or above EPA actionable level, and zero percent of the homes built after 1978 had such a sample. The mean test kit completion time is 23.25 minutes.

Conclusion: The study is still ongoing. Preliminary results from the study support the hypothesis that older homes, built before 1950, have elevated lead levels, with a decrease in lead from 1950-1978, and no lead after 1978. Further, participants have provided positive feedback and suggestions to improve kit usability. A prototype is being developed. In the future the kit is intended to be scaled up to benefit families from St. Joseph County, and, if possible, statewide.

Year Built	Percent of Homes with Lead
Pre-1950	100
1950-1978	42.9
Post-1978	0

Figure 1- The percentage of homes from each time period with at least one sample of lead greater than EPA hazard standards.

Optimization of antimicrobial activity of truncated linear variants of enterocin AS-48

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With the growing threat of antibiotic resistance in bacterial species, antimicrobial peptides (AMPs) have the potential to act as alternatives to traditional antibiotics. Bacteriocin AS-48, derived from Enterococcus sp., has been shown to have antimicrobial activity against a range of bacterial species. As a strategy to optimize the antimicrobial activity of this peptide, 95 variants of a shortened enterocin AS-48 parent peptide were produced by modifying the original sequence with systematic amino acid substitutions to increase the amphipathic, hydrophobic, or cationic properties. After determining the minimal inhibitory concentration (MIC) of the parent peptide, the peptide library was screened for antimicrobial activity against Escherichia coli, Pseudomonas aeruginosa, and Streptococcus pyogenes. Of the 95 variants, four were found to have significant activity against all three organisms in the range of 8-16 μM. The secondary structure of the library variants was analyzed by circular dichroism and computer modeling, revealing that in the presence of SDS micelles, the peptides adopt an alpha helical structure. Ethidium homodimer assays were conducted to determine the cytotoxicity of the peptides against eukaryotic cells. With future study, our strategy suggests that natural peptides with antimicrobial activity can be modified such that they may exhibit greater potency against a broader spectrum of bacterial species and minimal cytotoxicity to eukaryotic cells.

A low-cost 3D-printed electrophoretic method for proteomics sample preparation

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Mass spectrometry based proteomics has emerged as the dominant technique for quantitative protein profiling and identification due to technological advances in identification and quantitation that can be obtained from a single analysis with modern instrumentation. Conventional analysis of a complex proteome requires significant sample preparation for high quality spectra; namely effective protein digestion and sample clean-up prior to HPLC-MS/MS separation and analysis. Enzymatic protein digestion, typically with trypsin, is the preferred method for sample preparation; it generates thousands of peptides which are highly amenable to chromatography and MS-MS/MS analysis. Several laboratory and commercial techniques exist to improve the yield and suitability of protein-trypsin digestions for MS/MS analysis including in-solution digestion, filter-based, and in-gel electrophoretic methods, most notably SDS-PAGE. In gel preparation and digestion has the advantage of excellent removal of contaminants, and effective denaturation of proteins prior to proteolytic digestion. In gel digestion, however is adapted from slab-gels which were designed a priori for visualization and blotting, not mass spectrometry based sample preparation. Therefore, a low-cost platform offering sufficient protein cleanup through detergent and macromolecule removal with modest resolving power was developed for rapid sample preparation for conventional bottom-up proteomics. 3-Dimensional Tubular Acrylamide Gel Electrophoresis (3D-TAGE), a modular technique for protein separation using low-cost 3D printed technology, is presented as a robust, rapid, and approachable method for in-lab and field preparation of complex protein samples prior to bottom-up proteomics via HPLC-MS. This technique permits 30-minute separations prior to conventional tryptic digestion/desalting with protein loading capacities greater than 200 µg and a total build cost of under $10. Whole cell E. coli lysate prepared through 3D-TAGE, SDS-PAGE, and in-solution digest demonstrate complementary protein separation and peptide identification through Orbitrap MS-MS/MS based identification. The low-cost design combined with rapid separations and high compatibility with conventional proteomics techniques suggest that 3D-TAGE could be utilized as a preparatory platform for bottom-up proteomics in both typical laboratory workflows and low-resource settings.

Phosphate Detection Using Yeast Produced CO2

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Eutrophication is a term describing an excess of nutrients in the ecosystem which permits the unchecked growth of aquatic microorganisms, specifically algae. This runaway growth is often referred to as a bloom. Though both nitrogen and phosphorus may cause algae blooms, freshwater eutrophication is usually caused solely by phosphorus. When algae blooms occur, there are many consequences including the production of toxins, deoxygenation, fish die offs, and degradation of recreational waters. Currently, the primary methods of determining the phosphate concentration in water require hazardous and time consuming chemical tests. Our lab has been researching alternative methods of determining the phosphate concentration using yeast as a biosensor of which this study is an extension. These alternative methods work on the principle that yeast growth, as measured by optical density, is linear with phosphorous concentration. These methods have limitations on samples with colored and muddy water which is common in nature. This study investigates whether measuring the CO2 produced by yeast using a Nondispersive Infrared Sensor (NDIR) can measure phosphorus concentration in turbid water samples. The primary hypothesis of this study is that CO2 will have a linear relationship with the yeast growth. If this is true, then the CO2 concentration can be correlated to the amount of phosphorus in the system. Our data indicates that CO2 can report increases and decreases with yeast concentration, but a predictable relationship is thus far unclear. There is a consistent relationship between the CO2 produced and the amount of yeast in the culture, but more work will need to be done to quantify this relationship.

Can personality influence how you manage a social network?

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College students with larger networks tend be extroverted, and consequently have lesser depressive symptoms. Despite this, there is a dearth of research on how extroversion levels can impact the management of a network. Can the mismanagement of a network cause depression, and can extroversion – or lack thereof – play a significant role? The current study sought to address this question with 3 hypotheses; (1) can extroversion predict network size, (2) can depression scores predict extroversion and network size, and (3) can a variation in network size due to extroversion attribute to depression scores. For this study, researchers utilized the Net Health data set, which included behavioral and network data from a large (n = 714) majority Caucasian (65.6%) sample of college students from a private religious Midwestern university. A simple, and multivariate linear regression were conducted to test these hypotheses. Residuals were used to assess the variation of network size due to extroversion. There was a positive significant effect found between the residual term and extroversion ($b = 0.972$, $p = < .001$), which supported the hypotheses. This research suggests that limiting a social network may benefit a college student. For college students who are introverts, there is an apparent need for them not overemphasize friendships, as this may create additional stress which could hinder academic performance.

An Analysis of Intellectual Property Diffusion in Global Markets

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The diffusion of innovation through intellectual property in global markets has significant impacts on economic growth and development. Governments intervene in the innovative process by investing in research and development as well as protecting inventor's rights through patent systems and intellectual property treaties. In this work, we analyze global trends and distributions of patent applications domestically and abroad by comparing and contrasting major patent offices. Specifically, we examine the impact of patent systems on patent quality and quantity by analyzing the recent change in the U.S. patent system through the America Invents Act of 2011. In conclusion, we highlight specific trends which may positively or negatively influence the diffusion of intellectual property in relation to GDP growth.

Advancing the Tools for Global-Scale Computational Social Science.

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We introduce the Global Open Simulator (GOS), a library for computational social science models written in Python and designed for Jupyter. Using a subset of known social and economic factors, we demonstrate the system using a model for global migration. We show the challenges of managing datasets, implementing flexible formulas, and visualizing outputs and display how GOS is able to simplify these tasks. Finally, we speculate how these tools can be used to bridge computation models and social science datasets with a global perspective.

Developing Software to Process Malaria Genetic Data for QTL Analysis in a Shared Parent Genetic Cross

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Our current understanding of the genes responsible for drug resistance in human malaria has largely relied on Quantitative Trait Locus (QTL) linkage analysis of genotype-phenotype data derived from three genetic crosses using chimpanzees as the stand-in host for a human. While these crosses revealed information about the malaria genome, their power for discovery was hindered by the biparental design, which introduces sampling bias. Since the recent ban on chimpanzee research, a new method for performing genetic crosses in malaria has been developed using mice with 'humanized' livers. This method provides new opportunities to determine the effects of malaria genes on complex phenotypes, such as drug resistance. Several new crosses have been generated using this methodology, including two crosses that share a parent. The progeny were sequenced with Illumina Next-Gen sequencing and genetic variation among the progeny was captured using single nucleotide polymorphism (SNP) variants. I developed a software pipeline to analyze the SNP data and identify unique clonal progeny lines that contain no missing data. I then developed software to perform QTL analysis in a shared parent population (2 different crosses with one parent in common). This approach provides more phenotypic diversity and provides greater statistical power to detect genes with small effects.

SNP Isolation and Primer Design in R. pomonella

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The apple maggot fly, Rhagoletis pomonella, has threatened the apple industry of the Pacific Northwest (USA) by laying its eggs into apples since the fly's introduction to the region around 1980. The species has cost the industry approximately $8 million annually in recent years; therefore, monitoring and preventing further spread of R. pomonella throughout this region is critical. These endeavors have proven difficult, as there exists another species, R. zephyria, which is morphologically identical to the apple maggot fly, yet presents no harm to apples. In my research, I integrate a well-researched file containing the draft genome of R. zephyria, as well as a compilation of single nucleotide polymorphisms (SNPs) that indicate differences between certain regions of the two species' DNA, with the goal of designing a cost-effective panel of diagnostic genetic markers to differentiate the two species. Isolating the SNP regions required creating primers, single strand DNA sequences necessary in PCR, which required the consideration of many factors for producing the most encompassing, primer-making algorithms. Further laboratory examination will narrow these computational predictions to a panel of approximately ten reliable diagnostic markers, which will allow farmers to efficiently differentiate R. pomonella from other harmless, yet similar looking species like R. zephyria and mitigate harm that this species inflicts on the apple industry.

Visual Analytics of Student Clickstream Data Using Higher Order Networks

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The ability to draw meaningful conclusions from sequence data can be useful for a variety of applications, including the study of DNA, worldwide shipping data, and web clickstream traffic. Sequential data can often be represented as a network, in which individual data points are denoted as nodes, with connections between them indicated by edges. In this project, we study the web clickstreams and grades for a particular course of students surfing Sakai (a virtual learning environment), across fourteen assignments, to extract the behavior patterns of the students and understand the relationships between the behavior and the grades. We develop a visual analytic system that incorporates an analysis component to establish the relationships and a visualization component to explore them interactively. We wish the system can assist instructors in identifying students at risk of failing assignments early, and assist students in learning from others to improve their study skills.

This dataset has been analyzed previously with a traditional first-order network (FON) representation, which does not take into account any higher-order dependency of clicks in the clickstream. We hypothesize that assigning a single website to each node in the network fails to encapsulate the complexity of the data. For example, a student who previews assignment questions before looking at study material is likely to perform better than one that does not preview questions. Thus a FON is insufficient to adequately analyze our dataset, and we must use an alternative approach. Recently, the higher-order network (HON) representation was introduced, overcoming this problem by assigning a sub-sequence of data points to a single node.

One major challenge resides in extracting compact patterns across the fourteen assignments: while two URLs assigned to different assignments are unique, they may be functionally the same -- e.g., both may be reading resources. We hypothesize that URLs that perform the same functional purpose should play a similar role in predicting grades, and propose that they would have similar structures in the HON. It would thus be beneficial to identify the structural identity of each HON node, and to use such information in our grade distribution predictions. For this purpose, we make use of struc2vec, a machine learning algorithm that generates a vector representation of structural identity for each node in the network.

The other challenge is how to intuitively present our results so that they can be interpreted by users unfamiliar with sequence data or HONs. To this end, we develop novel visualization schemes using the Javascript framework D3.js. Merging a sunburst diagram with a pie chart (creatively named a “sunpie”) allows us to easily compare student clickstreams, a task that would be difficult if we presented the data as strings of numbers. By linking our sunpie diagram with a force-directed graph, both color-coded according to the structural role, we provide an intuitive understanding of the HON structure.

Finally, in order to display the results of our grade distribution predictions, we combine a simple representation of the clickstream of interest with a Sankey diagram, allowing an in-depth exploration of the clickstreams that are most likely to lead to a particular grade.

Are all Personality Inventories Equal? Assessing the Applicability of the BFI-2 to Adolescents

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This research was conducted to investigate whether the Big Five Inventory 2 (BFI-2), a revised version of the original BFI, can accurately measure the personality of high school students. The BFI-2 was developed in order to improve the bandwidth, fidelity, and predictive power, while maintaining the reliability and validity established in the original BFI (Soto & John, 2016). This was achieved by implementing a hierarchical structure with three facets for each of the five domains. Soto and John (2016) validated the BFI-2 on an internet sample with mixed ages, and a college sample. This research examined whether the BFI-2 remains reliable and valid in the high school population using data collected from students enrolled in an AP statistics class from Indiana high schools. In this project we replicated the analyses in Soto and John (2016), including the alpha reliability, correlations between domains and facets, and exploratory and confirmatory factor analysis of the domain and facet structure. In addition, we investigated gender differences on responses to the BFI-2. Measurement invariance was also examined to test whether the BFI-2 accurately and equally measures both males and females. This work was supported by National Science Foundation grant SMA-1560089: "REU Site: Computational Social Science".

Deep Learning for Particle Physics: Investigating Neural Network Structure and Hyperparameters

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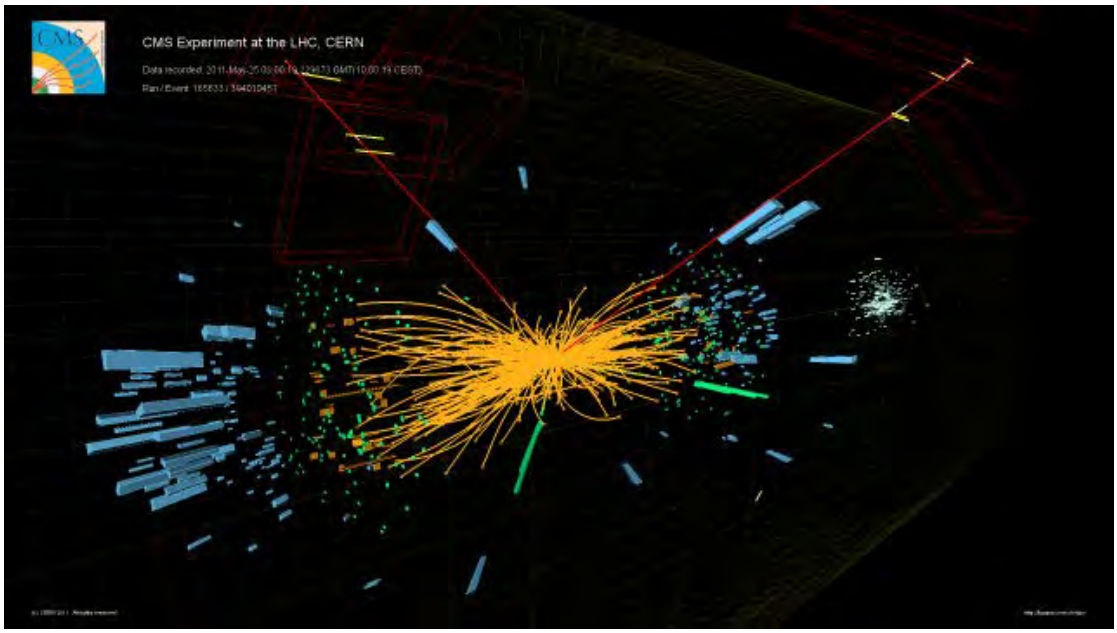
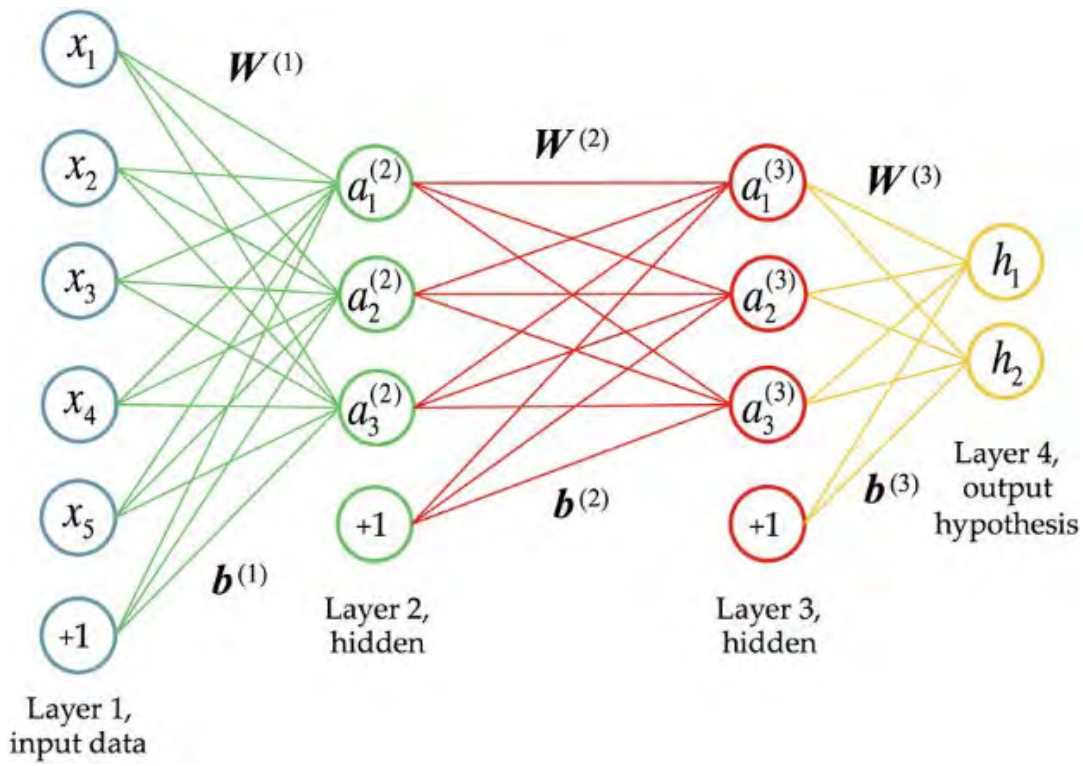
The Large Hadron Collider (LHC) at CERN is home to several experiments on the cutting edge of high energy physics, including the Compact Muon Solenoid (CMS) experiment. The accelerator collides proton beams with velocities approaching the speed of light and records the signatures of the resulting interactions. Studying certain exotic collisions has already expanded our knowledge of the standard model of particle physics and has the potential to further our understanding of elusive fundamental particles, such as the Higgs Boson. However, it is difficult to accurately classify scientifically interesting collisions and separate them from background signals, especially due to the level of ambiguity in reconstructing collisions from data. In addition, there are approximately 600 million collisions per second at the LHC, with a total data flow of 25 gigabytes per second, or 600 megabytes per second for the CMS experiment alone (1). This is far too much data for physicists to study, so it is crucial to improve data processing methods such that the collisions of interest can be identified for selection, and not the large quantity of background.

Deep learning methods are algorithms modeled after the brain that utilize multiple layers of neuron-like nodes to approximate the learning process. Although deep neural networks are a promising solution to particle physics' data challenge, they difficult to optimize, as traditional "black box" methods utilize learned parameters that don't necessarily correspond to intuitive variables. In order to harness fully the potential of deep neural networks for applications in particle physics, it is necessary to first understand how to optimize networks for performing simple operations relevant to this data and the effect of network hyperparameters and architecture on their overall performance. This project investigates methods of network construction, size, and structure to optimize networks for simple physics problems. These networks, designed with intuition for a particular problem, are then compared to black box type networks to test whether the added structure improves accuracy and utility.





(1) "Processing: What to record?" CERN, Aug. 2012, cds.cern.ch/record/1997399.

Utilizing a Bayesian Point Process Model to Predict Forest Fires from Charcoal Data

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Forest fires bring devastation to many people throughout the United States and the world. Air pollution and destroyed vegetation are two large consequences of forest fires, and these lower the standard of living for many people. As the climate warms, different kinds of vegetation will thrive which in part will create different kinds of fuel needed for forest fires to start which, as aforementioned, will create more air pollution. Better education of what causes these forest fires and different policies enacted by lawmakers provide for potentially less forest fires and better prevention. Our model, along with a climate model and vegetation information, create a “forest fire simulation” model, part of which is decision making by people.

The model we are using is a Bayesian Point Process model created by Malcom Itter, a post-doctorate researcher at Michigan State University. This model predicts changing fire return intervals over thousands of years using charcoal particles found in sediment cores of lakes. Charcoal particles build up in lake sediments after forest fires. The model distinguishes between two types of charcoal: a background intensity, which is a steady background charcoal influx due to regional fires and a foreground intensity, a more jagged signal created by local fires relative to the lake. The model is run for each lake individually (univariate model) and for all of the lakes in the region collectively (multivariate model). The multivariate model provides cross-lake information on background intensity, but the univariate model alone allows us to calculate the changing probability of foreground and background fire and as well as the mean fire return interval.

After validating that we could run and understand the model fit to the Alaskan data set, we applied and tweaked this model for a group of lakes in Minnesota collectively knows as the Big Woods lakes. Before European settlers, the Big Woods was a mixed region of savannahs and forests, which we expect had different fire regimes than Alaska. The Big Woods lakes are also closer in proximity to one another when compared to the Alaskan group of lakes. We ran the univariate model for Crystal Lake in the Big Woods dataset. Results suggest that wildfire in the Big Woods may be challenging to the model. The model for Crystal lake estimated high amounts of background charcoal, which could either correctly indicate high input of regional charcoal or the model could be attributing charcoal from frequent local fires to regional sources. We expect that running the multivariate model across the entire Big Woods dataset will provide better estimates of regional background charcoal of the region, and better constrain the foreground intensity of Crystal lake.

Knowledge Diffusion in the Global Automotive Industry

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Knowledge diffusion in global markets influences the evolution of industry sectors. We analyze the impacts of global knowledge diffusion in the automobile industry in 4 major markets (China, EU, US and Japan). Data for this research was collected from the United States Patent And Trademark Office (USPTO). The patent assignment records whose assignor and assignee were both leading automobile or automobile part companies were selected. We look at the variance of automobile market share as one variable potentially dependent on knowledge diffusion through patent assignment. We hypothesize that patent assignment shortens the gaps between automobile companies leading to more market share parity in major markets . In order to quantify the relationship between patent assignment intensity with change in market share, we calculate Pearson correlation coefficients. The results shows that the share of automobile market in US and China have significant correlation whereas there are no significant differences found in the EU and Japanese markets. Further analysis yields a trend that automobile brands from EU and China put more emphasis on domestic market whereas automobile companies from Japan and US actively seek opportunities internationally.

Reduction of Resources Consumption in Parallel Applications Using a Density-based Clustering Model

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Often times we find our users will ask for orders of magnitude too few or too many resources to run their parallel applications. It would be ideal to achieve a near-optimal number of resources the application runs. We provide a clustering model for discovering clusters in all tasks run in a process and calculating the ideal number of resources of each cluster.

The resource monitor was used to record computational resources of all tasks, and cores, memory, disk and wall-time in the reports were extracted to be used as features of tasks. Density-based data clustering was used to cluster all tasks and calculating the ideal number of resources of each cluster. After clustering, we obtain several clusters, then we calculate the maximum resources (cores, memory, disk) of each cluster and label all tasks with cluster numbers.

We ran experiments with a synthetic workflow of homogeneous tasks as well as the bioinformatiocs tools Lifemapper, hecil and Shrimp. The experiments were designed to capture the inherent nature of resources consumption of a parallel application, the clustering allowed by the model, and its usefulness in real applications.

Clustering model is able to save resources consumption when users need to run the same workflow for multiple times or run a small batch of database to obtain optimal resources allocation before running the whole large batch system.

Internal Representations of Interparental Conflict and Withdrawn/Depressed Symptoms: The Moderating Role of Mother-Adolescent Attachment

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Extant literature has shown that mother-adolescent attachment is predictive of the internalizing symptoms of withdrawal/depression (Rice, 1990). Additionally, it is clear that adolescents' internal representations and feelings of emotional security towards marital conflict are important to their adjustment over time (Davies & Cummings, 1994). However, limited research has investigated the interaction between parental attachment and emotional security. Due to the possibility of adolescents having secure parent-adolescent attachments, but insecurity in the family relationship and vice versa, it is important to consider the interaction between these two constructs. This study investigated the role of perceived mother-adolescent attachment as a moderator between adolescent's perceived emotional security, through internal representations, and self-reported withdrawn/depressed internalizing symptoms. The average age of participants was 13.26. The Inventory for Parent and Peer Attachment (IPPA), the Security in the Interparental Subsystem Scale (SIS), and the Youth-Self Report (YSR) were used to conduct a standard multiple regression analysis. Mother-adolescent attachment was a significant moderator, indicating mother-adolescent attachment serves as a buffer between high internal representations (emotional insecurity) and withdrawn/depressed symptoms. Findings support further investigation into the interaction of attachment and emotional security, and its prediction of psychopathology.

Infant and Child Mortality Rates and the Role of Female Education: A Meta-Analysis of Statistically Significant and Insignificant Research

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Infant and child mortality rate is considered an important indicator of a women's health status and maternal education has been widely used an indicator of socio-economic status. Every country has collected data on childbirth and sadly, child death. Over the past century, there has been an increasing amount of research on infant mortality rate and women education; however, while some studies show there is a consistent, statistically significant, negative relationship (more education = fewer deaths) between maternal education and infant mortality rate, other studies have shown the opposite. This research provides a meta-analysis of 42 scholarly articles that evaluate the relationship between infant mortality rate and maternal education. In the meta-analysis, we looked at the types of models scholars used, units of analysis, the conceptualization of the variable for women's education, the significance of the women's education variable, whether it was a panel data or if the women's education variable was skewed, whether there was a fixed effect or a random effect and more. As a result, we found that out of the 42 scholarly articles, 45.2% had shown consistent, statistically significant relationships, while 54.8% of the articles in our sample showed inconsistent or no statistical relationship. This could be because the articles with little to no significance used more comparison of education levels than the articles with relationships that were always statically significant. Additionally, the articles with little to no significance took more data at the individual level, while the articles with relationships that were always statically significant used more of a balance between a unit of analysis of countries and individuals. Lastly, the differences in outcome for many of the scholarly articles was the result of other variables taken into account including, but not limited to, urbanization. These are some of the factors that could have played a role in the way in which the data in the 42 scholarly articles were interpreted.

The Effects of Mandatory Retirement on Employee Health Outcomes

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The work environment provides important social and economic supports for employees integral to their overall wellbeing. As a result, some have expressed concern that mandatory retirement may be detrimental to health. In contrast, for many, work generates direct health risks and mandatory retirement can actually reduce mortality. As of yet, there is there is little work on the consequences of involuntary separation. This study looks at one such case, namely, the effects of mandatory retirement of commercial airline pilots on mortality. Up until 2008, Federal regulations required the mandatory retirement of commercial airline pilots on their 60th birthday. Using data from the 1980 Census 5-Percent Public Use Micro Sample and a regression discontinuity design model, we first demonstrate that the law forced the exit of 60 percent of pilots from the workforce in the quarter they turn 60. Using data that is a census of Pan Am pilots that worked for the airlines through the early 1980s, we use a regression-kink design to see whether there is a shift in the Gompertz-Makeham Law of Mortality curve (e.g., log-mortality is linear in age) at age 60. Results from this analysis show a significant downturn in the Gompertz-Makeham curve at age 60. In contrast, data from the National Longitudinal Mortality Survey shows no such shift in the Gompertz curve for other high-income workers.

Performing Black Masculinity

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According to William Darity, masculinity is “a socially constructed expectation of appropriate behaviors, beliefs, expressions, and styles of social interaction,” which rely on constant affirmation and approval from onlookers to be deemed authentically masculine. In other words, masculinity is a performance driven by the applause of an audience of everyday people. Men use their voices, clothes, gestures, and walking style to perform masculinity on a daily basis. Representations of ‘authentic masculinity’ are found all over the media. Rap lyrics tell men to be sexually promiscuous and use women’s bodies as sport; movies tell men that wielding a gun and being overtly muscular are desirable and manly; and television tells us that homosexual male characters must be supporting roles. In order to sell the image of masculinity, media representations have to eliminate anything that challenges the socially constructed ideal of hyper macho masculine men.

While popular music and television function to subconsciously frame Black masculinity, live theater serves as a space that forces audiences to critically think about what is being presented to them. Further, the special intimacy of the theater is conducive in allowing people to listen to what others have to say, an act that may not occur in any other setting. As one sits in the theater, you theoretically have no choice to change the station, look to your phone for comfort, or walk away from discomfort. Within such a space, it is critical that the work placed on stage provides accurate and diverse representations of characters.

This project explores the ways Black masculinity is constructed by actors, writers, and directors in popular culture and theater. The texts and images examined in this project illuminate the methods used to perform Black masculinity and the effects such performance has on the framing of understandings of Black manhood.

Light Activated Synthesis of Au Nanoplates

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Grad Student or Postdoctoral Mentor: Spencer Golze

Improving the quality of life requires innovations in science, medicine and engineering. Gold nanoparticles (Au NP) have generated interest due to unique properties that allow for their use in optical and electronic applications. Some of the applications of interest include Surface-Enhanced Raman Spectroscopy (SERS), catalysis, electronic conductors, and the localized treatment for cancer cells. The opto-electronic properties of these Au nanostructures are heavily dependent upon morphology as well as the overall size. Currently, there is interest in the development of planar hexagonal and triangular Au structures because this geometry is well-suited to plasmonic, electronic, and medical applications since the plasmon wavelength can be varied widely by changing its size and the fact that gold is biocompatible. This study entails synthesizing these planar Au NPs by fabricating gold seeds in aqueous solution and subsequently exposing them to a white light source that preferentially promotes growth on certain crystal facets due to a light-mediated process. An electron microscopy study was performed utilizing an FEI Magellan 400 Scanning Electron Microscope to investigate the planar growth of these colloidally fabricated Au nanoplates. The goal is to provide a direct comparison to similar structures formed on substrates that have been produced in our lab using epitaxially mounted Au seeds positioned in an array.

A second aspect of this study was to make improvements to the experimental set-up used to synthesize substrate-based planar structures. The current setup is conducive to a specific set of parameters, but improvements will allow for investigations of different aspects such as the variation of solution temperature, filtered wavelengths of light, and precise positioning of the substrate during growth. To allow this, an optical stage has been designed that contains optical elements such as filters and polarizers, improved consistency and control, and the ability to heat the growth solution to increase the growth reaction rate. The proposed changes to this experimental setup should result in a more consistent growth, a wider range of accessible growth parameters, and an overall improvement to the synthesis of these nanoplates.

Feasibility of Vehicle-Wake Energy Extraction by Roadside Wind Turbines

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Increasing public awareness of climate change and existing methods of power generation has been accompanied by a rising interest in renewable energy. A popular method of renewable energy generation is wind energy, which is most recognizable by 100-meter tall horizontal axis wind turbines (HAWTs). However, the benefits and uses of smaller vertical axis wind turbines (VAWTs) are continually being explored.

The purpose of this study is to determine the feasibility of utilizing energy from the wake of passing vehicles on a highway for the electrical generation of power, via roadside VAWTs. Some VAWTs claim to be “self-starting” turbines, meaning once a specific minimum wind speed has been reached (the cut-in velocity), the turbine will begin to move, and thus generate power. Therefore, it is necessary to establish the height and distance from the road at which the wake of a vehicle is sufficient to generate power from a VAWT.

Wake measurements for a scale-model semi-truck were taken in a small wind tunnel using a pitot static probe system, with the wind speed at approximately 27 m/s. Regions of wake behind and alongside the scale model were analyzed to document the air velocity at several heights. The collected data was processed to create velocity maps representing the air velocity at many individual points around the model, enabling us to determine the cut-in velocity requirement for a turbine at one width separation from the model.

The results of the wind tunnel test indicate that the largest wake is generated at approximately 75% of the model’s height, and that the magnitude of the wake decreases as distance from the center of the truck, in the widthwise direction, decreases. The data also suggests that the magnitude of the wake increases (at least for small widthwise distances) as distance behind the model increases. Technical specifications from commercial VAWT manufacturers claim cut-in velocities as small as 1.3 m/s for their turbines. Our wind tunnel tests measured wake between 1.5 and 3.0 m/s at a relevant distance from the model, suggesting that the wake from a vehicle may be sufficient to generate power from a self-starting VAWT.

Future phases of this project will include the implementation of a VAWT along the I-80 Indiana Toll Road, in collaboration with our sponsor, the Indiana Toll Road Concession Company LLC (ITRCC). The ND-ITRCC Highway Wind Turbine, along with a small

meteorological tower, will be monitored by a team of Notre Dame undergraduates and an advising faculty member for a period of 6 months, with the goal of verifying our results from the wind tunnel tests and observing the performance and condition of the turbine.

VASP Calculations and Reactor Design for Ethylene Oligomerization

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Grad Student or Postdoctoral Mentor: Galiya Magazova, Neha Mehra,

Our research is to figure out the most promising catalyst for performing ethylene oligomerization. Zeolites are known for their catalytic role in olefin oligomerization. Experiments are done to synthesize MCM-41(Mobil Composition of Matter No. 41) using different Si/Al ratios. One of the techniques of characterization is physisorption, which tells us the surface area and pore sizes of the zeolite. We used the flow reactor to test the catalyst. Using a GC-FID (Gas Chromatography-Flame Ionization Detector), we are able to identify the products obtained from the reaction. In computation, we are computing the reaction energy of ethylene binding onto CHA (Chabazite) zeolite. It is computationally easier to study CHA zeolite over other zeolites because it has a single type of T-site. Jupyter Notebook is utilized for coding the calculations in python. VASP is needed to perform the density functional theory (DFT) calculations on reactions and model systems. VESTA helps to visualize CHA zeolite and inspect T-sites providing right geometry of structures for computations and their analysis. The results from experimental and computational studies provide strong starting points to further elucidate the catalytic cycle and the most efficient catalysts for ethylene oligomerization.

Synthesis and characterization of iptycene-based polyimides with tunable chain rigidity for gas separation membranes

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Faculty Advisor: Dr. Ruilan Guo
Grad Student or Postdoctoral Mentor: Qinnan Zhang

This research focused on synthesizing polymers and utilizing their different structures to create films used in gas separation studies. Polymer films provide a more environmentally friendly, durable option to the thermally driven processes used by industries currently. Specifically, iptycene-based polyimides show outstanding gas separation performance according to many studies. The intrinsic rigid structure of polyimides and bulky iptycene units disrupt the efficient polymer chain packing, providing high fractional free volume and allowing fast gas diffusion through the polyimide membranes. My project focused on synthesizing a novel triptycene-containing polyimide for small gas separation. Triptycene-direct diamine (TPDAm-d) and triptycene-based dianhydride (TPDAn) -monomers with high purity were prepared and combined to form a polyimide using the chemical imidization method. However, the challenge with this reaction is the low solubility of the polyimide. The combination of TPDAm-d and TPDAn yields a highly viscous solution of a poly(amic) acid, indicating good reactivity of the first step. During the chemical imidization step where pyridine and acetic anhydride are added, the product tends to precipitate out during the reaction and gelling of the solution occurs, indicating too high molecular weight or even cross-linking of the polymer. This prevents complete imidization of the final product and causes difficulties collecting the polyimide. Moreover, the product is difficult to dissolve in common solvents and therefore hard to cast a film. Therefore, different reaction conditions and methods were tested to solve this solubility issue. Altering the procedure to slow down the reaction was done by adding an ice bath during the chemical imidization step. In addition, adding the pyridine and acetic anhydride in long time increments was done so that the viscosity of the solution could be monitored and more solvent could be added if the reaction appeared to be gelling. Different solvents were also tested focusing on dimethylacetamide (DMAc) and 1-methyl-2-pyrrolidinone (NMP). Despite these additions, gelling has still occurred to some extent creating a polyimide that is difficult to dissolve for the film casting step. The remaining weeks of my research will focus on trying to prevent gelling during the reaction by varying reaction conditions, adding functional groups that can improve solubility of the structure, and creating films that can be tested for their gas separation capabilities.

Development and Characterization of Plasma Catalytic Reactors

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Other Contributors: Pritam Nayak

The ionized gas in non-equilibrium plasmas is a highly reactive medium, containing a wide variety of charged and neutral reactive species. When coupled with catalytic materials, synergy between plasma and catalyst has been demonstrated for various reactions, including dry methane reformation, carbon dioxide dissociation, and even ammonia synthesis. There are two predominant propositions for this synergetic enhancement: the plasma enhances catalytic activity by adding local energy to the catalyst and producing excited species that readily react with the catalyst, or that the catalyst alters the plasma itself, making it more reactive and enhancing chemical processes in the plasma. In this work, the effect of metal catalysts on the macroscopic electrical characteristics of a non-equilibrium plasma generated in a dielectric barrier discharge reactor for the synthesis of ammonia (NH3) from nitrogen (N2) and hydrogen (H2) is examined. The macroscopic electrical characteristics of the plasma were observed for multiple different packed bed materials, including Al2O3 (alumina) support, and metal-support mixes of Fe-Al2O3, Ni-Al2O3, and Co-Al2O3; these mixes ranged from catalytically ineffectual to effective, respectively. Multiple gas ratios of (N2:H2) were studied, and the packed bed length to electrode length ratio was varied, while the plasma power was scaled by volume. The electrical characteristics investigated include the capacitance of the reactor cell measured from Lissajous plots, and an analysis of the plasma current for peak number and average peak height and width. Over all conditions of equal power and gas ratio that were tested, no statistical differences in the electrical properties between any of the metal-support catalysts were found, though conversion for each set of experimental conditions changed with the catalyst. These results support the argument that any observed synergy is not due to the catalyst enhancing the plasma, but due to the plasma changing the catalytic activity of the catalyst. The likelihood that no significant electrical differences exist among the support and support-catalyst powders provides further motivation for an experiment investigating the effect of the plasma on the catalyst using in situ surface chemistry measurements.

Synthesis and Characterization of Platinum (II) Carbene Complexes

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Transition metal carbene complexes have become an area of great interest in catalysis and small molecule activation. A square planar platinum(II) carbene complex [{PC(sp2)P}HPtPMe3] ([PC(sp3)H2P]H = (bis[2-(di-isopropylphosphino)phenyl]methane) was synthesized through the dehydrohalogenation of [{PC(sp3)HP}HPtCl] in a microwave reactor. An analogous complex, [{PC(sp2)P}tBuPtPMe3] ([PC(sp2)P] tBu = bis[4-(tert-butyl)-2-(di-isopropylphosphaneyl)phenyl] methylene) was synthesized via a similar route. The nucleophilic nature of the carbenic carbon was determined through DFT calculations and further reactivity studies are currently being conducted to confirm this. The platinum carbene complex was one-electron oxidized with I2 to form [{PC(sp2)P}HPtI], a persistent radical species. This paramagnetic complex is currently under further investigation and characterization.

Coordination Chemistry of the Human Copper Transporter

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Other Contributors: Dr. Steven Corcelli, Shelby Brantley

Copper, a transition metal, acquired through diet and then transported to proteins, cells, and organs, is important to human health. A dysregulation of this metal in the human body can lead to neurodegenerative disorders such as Alzheimer's disease, Parkinson's, or other diseases including osteoporosis. Copper is brought into cells by copper transporter 1, Ctr1; therefore, the study of this transporter protein is essential in the understanding and function of copper in the body. In this study, using computational chemistry, the first 3 amino acids of Ctr1 which are MDH, will be studied including a mutation of the second position to MNH, MAH, MEH, MGH, MQH, MDab (diaminobutyric acid), and MDapH (diaminopropionic acid). These mutations could help to understand the significance of this position and how the difference in the second position amino acid affects the binding of copper. With the assistance of various computer software, density functional theory calculations, single point energy calculations, and energy calculations without copper bonded to the protein, will provide more information about the energetics of copper binding.

Synthesis of transition metal alumosiloxide complexes as models of zeolite active sites for energy-related catalysis

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Transition metal ion-doped zeolites can facilitate a number of interesting reactions, including C-H bond activation. However, the mechanisms of these reactions and the structures of the catalytic active sites are not fully understood. We aimed to synthesize molecular mimics of transition metal zeolite active sites to study these fundamental questions. We targeted 10- to 12-membered alumosiloxane or alumosiloxide macrocycles as appropriate ligands for transition metal ions like copper or iron. These structures were approached using a few different synthetic routes. In one, copper siloxide complexes were prepared from 1,1,3,3-tetraphenyldisiloxanediol and copper(II) chloride. Current structures have ligands including lithium-pyridine bonds and lithium-tetrahydrofuran bonds, but to better mimic zeolite structures, reactions to exchange the lithium centers have been attempted using compounds such as aluminum chloride and aluminum isopropoxide. A second route has targeted the synthesis of salen, salen-like, and diketiminate ligands as ancillary ligands on aluminum. Current work includes functionalization of the aluminum complexes with siloxide substituents.

Synthesis of Nickel Phosphide on Aluminum Oxide

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Noble metals are widely used for catalytic dehydrogenation of light alkanes. Nickel phosphide (Ni2P) is a promising replacement of the current noble metal catalyst. Here we report the synthesis and characterization of a Ni2P catalyst on aluminum oxide. We used incipient wetness as well as temperature programed reduction to synthesize the catalyst. We have used nitrogen physisorption to find the surface area, average pore size, and total pore volume of the Ni2P catalyst on aluminum oxide. We optimize the crystal structures of Ni2P with density functional theory calculation. The optimized lattice constants are in agreement with literature. We have successfully prepared and characterized the Ni2P. The catalyst will be used for alkane dehydrogenation, which is the first step in converting shale gas into transportation fuels.

Computational Identification of Anharmonic Vibrational Frequencies for Brønsted Acid Sites in Aluminum Substituted Chabazite

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One of the missions of CISTAR is to improve oligomerization of light olefins and hydrocarbons. Zeolites play an essential role in the catalysis of these processes. This research is focused on using density functional theory (DFT) to better understand the Brønsted–Lowry acid sites in aluminum substituted chabazite (CHA) zeolites. In a single-aluminum substituted CHA, there is one isolated acid site with four distinct oxygens the proton can bind to [1]. One method for characterizing these acid sites is infrared spectroscopy (IR). Each of these proton locations has varying probability and contributes to the observed IR spectrum differently. The DFT simulations assume that molecules fit a harmonic model when calculating vibrational frequencies. The vibrational frequencies calculated for each of the four acid sites exceed experimental data by approximately 103 cm-1 [2]. A portion of this difference can be attributed to the harmonic approximation. To identify the anharmonic correction factor, the proton was manually moved along the trajectory found by using the harmonic model. At each point, the potential energy of the structure was obtained. Using these points, the Schrödinger equation was numerically solved in one dimension to identify the possible energy states, and ultimately anharmonic vibrational frequencies. The weighted average anharmonic correction factor was 171.4 cm-1. The experimental IR spectrum is likely the result of the contribution of paired sites, so the same method can be extended to aluminum pairs in CHA. With aluminum pairs there are two OH stretch frequencies present. The energy weighted average anharmonic correction factor was found to be 165.6 cm-1. This shows that the harmonic model over approximates the experimental consistently. The anharmonic correction brought computational findings closer to experimental but not precisely. This shows that other assumptions made in the DFT calculations contribute to the incongruent simulated and experimental data.

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[2] Smith LJ, Davidson A, Cheetham AK. A neutron diffraction and infrared spectroscopy study of the acid form of the aluminosilicate zeolite, chabazite (H- SSZ-13). Springer. 1997 Oct 7 [accessed 2018 Oct 17]. https://link.springer.com/content/pdf/10.1023/A:1019097019846.pdf

Synthesis and performance testing of pentiptycene-based polymeric membranes for mixed gas separation

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Polymeric gas separation membranes provide an energy-efficient alternative to competing separation processes such as cryogenic distillation, pressure swing adsorption, and chemical absorption processes used to separate common industrial gas mixes [1]. These membranes use their micropores to sieve gases according to their size, and their interactions with the polymer structure. Although there are several types of polymers in use industrially, polymers of intrinsic microporosity" (PIMs) are promising because they utilize their highly contorted and rigid polymer backbones to intrinsically introduce voids in the polymer through inefficient chain packing in the solid state [2]. This project focuses on the development, synthesis and testing of a novel pentiptycene-based monomeric series that can be used to make polymer films capable of demonstrating competitive gas-separation performance. The pentiptycene monomers are synthesized from cheap, widely available precursors, and in the synthetic process, two isomers of the monomers form: the C-shaped and S-shaped monomers. We have successfully designed and implemented a synthetic pathway that yields high purity monomers for both isomers and have film-casted co-polymers with PIM-1. Future research will focus on performance testing our co-polymers, and the development of more polymeric series where the center-ring substituents can be varied to finely tune gas-separation properties.

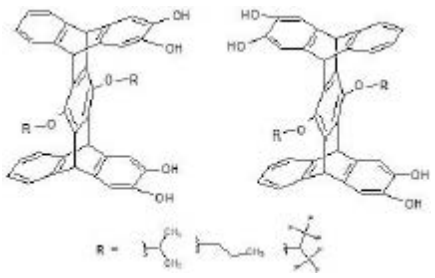

Figure 1: Tetramethoxy pentiptycene (TMP-C/TMP-S) monomers with R representing center-ring substituent groups currently being studied

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Targeting therapeutics through supramolecular affinity

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The ability to selectively target therapeutics in the body remains a challenge. One potential solution is to combine two powerful tools, metabolic glycoengineering (MGE) and supramolecular chemistry. MGE uses unnaturally modified sugars to introduce chemical signatures onto cell surfaces. Supramolecular chemistry uses specific, dynamic, and tunable non-covalent recognition interactions. Although MGE and supramolecular chemistry have both been extensively used for cancer diagnosis and therapy, they have not previously been applied together. In this project, we propose designing a new sugar derivative bearing a supramolecular ligand, which can be metabolized and presented on cells. We also synthesize a corresponding host conjugated to a reporter. Through exploiting host-ligand recognition, we intend to drive payload to the cell surface. This strategy can be further expanded to the delivery of drugs, diagnostic imaging agents, or agents for immunotherapy.

Stretchable Polymer Composite Film with Extreme Ductility and Toughness

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Other Contributors: National Science Foundation(1706039), Naughton Foundation

The purpose of this project was to create a polymer composite material with great ductility yet high tensile strength. It is uncommon for a material to exhibit both of these properties, as high strength is generally accompanied by a low ductility. However, the possible combination of these two properties is desirable as it would allow for a material to undergo significant strain without the risk of failure. This would be especially useful in the area of flexible electronics as it would allow for the development of reusable devices. Therefore, the focus of this project was to develop and optimise a procedure which would allow for the extreme flexibility of PDMS film to be combined with the high tensile strength of molecularly aligned polyethylene films.

Polydimethylsiloxane (PDMS) is a silicone polymer that is widely used for the production of microfluidic chips due to its low cost, durability and biocompatibility. In this instance, PDMS film was used as the bulk material in the polymer composite due to its great ductility and flexibility. The polymer composite acquired its strength by reinforcing the PDMS with aligned polyethylene films. Prior research has shown that detangling the polyethylene micro-structure to produce aligned chain of molecules can increase the tensile strength of polyethylene in the chain-length direction beyond that of steel, while maintaining its bending flexibility. This, along with the low cost, made polyethylene the ideal material to be used as the reinforcing material in the polymer composite developed. However, polypropylene (PP) films were more commonly used in the development stage of the polymer composite due to the fact that it is more widely available.

The manufacturing process consists of sandwiching a specified number of PE film ribbons between two identical stretched PDMS films, each with a thickness of 100 μm. The two stretched films were permanently bonded using the corona treatment and, upon relaxation, the PE film formed distinct wrinkles in the PDMS film that allowed for great flexibility with much improved strength. In order to successfully implement this manufacturing procedure, it was necessary to design a device which would ensure that the two PDMS films were stretched by the same amount and held in that position for the entire curing process.

Overall, the manufacture of the polymer composite was successful whereby highly flexible films were developed with a much greater strength. However, further testing would be

required in order to improve the quality of the films produced and to ensure their consistency. With an improved method, it may be possible to produce larger samples of the polymer composite or develop an automated process. In addition, further research is currently being carried out in order to find a way to reinforce the polymer composite in two directions by inventing a two-way stretching device for the PDMS film.

Development of Microimplants for Deep Tissue Optical Sensing

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Although treating cancer using a personalized medicine approach is widely discussed with great excitement, treatments for cancer are still largely based on broad categories such as stage, grade, and molecular subtype. Monitoring tumor response to guide therapy in real-time is one way of delivering a personalized treatment. In this work, we develop a micro-implantable monitoring system that provides real-time feedback to therapy. There are no sensor technologies currently available that are capable of monitoring targets deep within the human body while remaining unobtrusive and functional. The device proposed here will be capable of monitoring deep tissue (> 1 cm) whilst being small enough to fit into a needle to be injected directly into the tumor. The device uses light to assess the optical properties of the tumor microenvironment. Sources of contrast can be endogenous (such as hemoglobin or water concentrations) or externally administered (such as a fluorescent dye), and can reflect the composition and metabolism of a solid tumor. The implant consists of one or more laser diodes, a photodiode, a radio-frequency power-harvesting circuit, and a Bluetooth microcontroller. The microcontroller is programed to take measurements in predetermined time intervals. This summer we have designed and constructed several printed circuit board layouts for the microimplant, programmed and communicated with the microcontroller over Bluetooth and designed and constructed both a trans-impedance photodetector amplifier circuit and a bias circuit for our laser. We also used an impedance analyzer to evaluate RF power harvesting coil designs, and tested our laser and detector in a series of tissue-simulating phantoms that mimic the optical properties of normal tissue and solid tumors.

Extra-pair Parentage in Field Sparrows (Spizella pusilla)

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Extra-pair parentage (EPP) occurs when socially monogamous male and female birds mate outside of their social pair, resulting in young that are not genetically related to one of the parents. EPP may occur either when females engage in copulations with males outside of their social pair, or because of intraspecific brood parasitism (IBP) when females lay their eggs in nests belonging to other females of the same species. Both extra-pair paternity and IBP may influence reproductive fitness by reducing the costs of parental care. In this study we investigate rates of EPP in Field Sparrows (Spizella pusilla). Breeding pairs of Field Sparrow were captured, bled, and color banded at St. Patrick's County Park in South Bend, IN in June and July 2018. Banded adults were observed to establish social pairs and locate nests. Blood samples were taken from 23 social parents and potential extra-pair mates. We found 8 nests and obtained genetic samples from 18 offspring. Each individual was genotyped at six microsatellite loci to determine parentage. Offspring not sharing alleles with the social father or mother were determined to be the product of extra-pair paternity or IBP, respectively. These results will contribute to ongoing research on EPP, IBP, and their effects on fitness in shrubland birds.

Modeling Equilibrium Reactions with Origin

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One of the rising challenges in an increasingly digital world, is that future scientists and researchers may not be equipped to respond to the rapidly changing industrial and research landscape. Few individual experts within their respective fields create computer programs that can potentially aid their peers with analyzing and collecting data. When scientists and researchers rely on previously developed software, they often find these programs either difficult to learn, out of service, or costly. Our research demonstrates the value of interdisciplinary education in the sciences, mathematics, and computer programming. We collaborated with the Haas Lab in the Chemistry Department at Saint Mary's College, to analyze data on copper interactions with the human copper transport protein (Ctr1).

Creating a Catalog for Albendazole Paper Analytical Devices

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Other Contributors: Aubrey Houser, Dr. Matthew Becker, Dr. Toni Barstis

The PADs (Paper Analytical Devices) project is a collaboration between researchers at the University of Notre Dame and Saint Mary's College. The project is designed to help people in developing countries know if their medicine is counterfeit or underdosed. A PAD, itself, is an index card sized piece of paper containing lanes preloaded with chemicals. A sample of a pill is crushed and applied to the PAD, which is then dipped into water. The water travels up hydrophilic lanes and carries pharmaceutical ingredients with it. The water and ingredients react with the chemicals on the PAD creating indicative color changes that allow for the detection of a chemical present in the medicine.

The image analysis group at Saint Mary's College is working to create catalogs of known PAD images. Our ultimate goal is for an untrained person to use a PAD, take a photo, and upload the photo through an app on their phone. After comparing the new image with older, known PAD images, the program will tell the user if their medicine has been detected. Our goal this summer is to create a catalog of images for the program. During this process we are exploring what makes a good catalog and how to refine the catalog so it produces minimal false results.

A set of images from field tests taken in the summer of 2016 on Albendazole (used to treat parasitic worms) have been visually verified for any presence of Albendazole. This summer we have run these images through an analysis program, which determined if the color of interest corresponding to the active ingredient was present. This was done by detecting pixels containing the correct color, teal blue, in the regions of interest. If there were fewer than 500 pixels of the correct color detected, the reaction was considered negative. If there were more than 500 pixels detected, the reaction was considered positive. The next step was to refine the catalog to eliminate false results by changing the acceptable number of pixels and deleting catalog entries that were unsuccessful or otherwise redundant.. After the catalog was refined, the percent of true positives and negatives increased. We will discuss our results from this test using existing Albendazole images and provide guidelines for improving a catalog.

Quantifying the Relationship between the Gut Microbiome and Blastocystis in Long-tailed Macaques

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Grad Student or Postdoctoral Mentor: Chissa Rivaldi and Benjamin Gombash
Other Contributors: Bailee Egan

Long-tailed macaques (Macaca fascicularis) are known to carry Blastocystis, an enteric protozoan parasite, often associated with Irritable Bowel Syndrome in humans. Studies have found Blastocystis infection to be correlated with certain bacterial microbiota in the guts of humans, for example Streptococcus, Prevotella, and Ruminococcus. Therefore, we wanted to explore these relationships in more detail using a non-human primate model system that shows more variation in Blastocystis infection across sites in Singapore. Literature suggests that Blastocystis interacts with the prokaryotic microbiome through indirect competition for resources or through direct predation of gut bacteria. Macaque fecal samples were collected from five different populations across Singapore. Bacterial microbiome data were characterized by 16S rRNA gene sequencing, and Blastocystis prevalence was measured using both 18S rRNA gene sequencing and microscopy of fecal smears. Microbiome data were analyzed alongside 18S sequencing and microscopy data for Blastocystis at the population level using Spearman correlation tests and general linear models to determine associations between Blastocystis and the Firmicutes-Bacteroidetes (F/B) ratio – an indicator of gut community composition stability and overall health-and specific bacterial taxa previously shown to be associated with infections in humans. Contrary to our predictions based on the literature, no significant associations were found between Blastocystis and the F/B ratio nor any of the specific bacterial taxa tested. Our results are discussed in light of additional analyses and approaches that can be used to explore these relationships further in the future.

RadioHound: A low cost spectrum sensor

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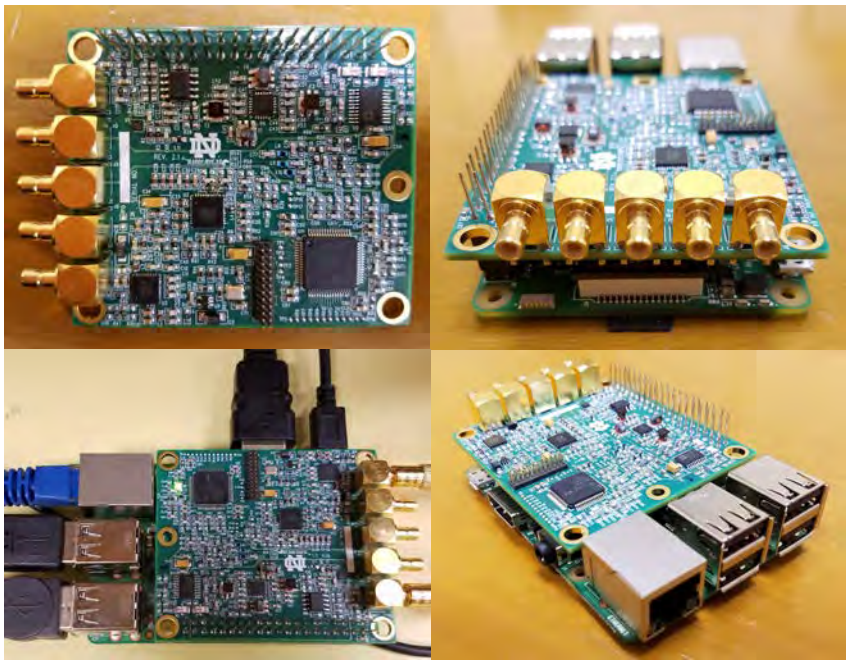
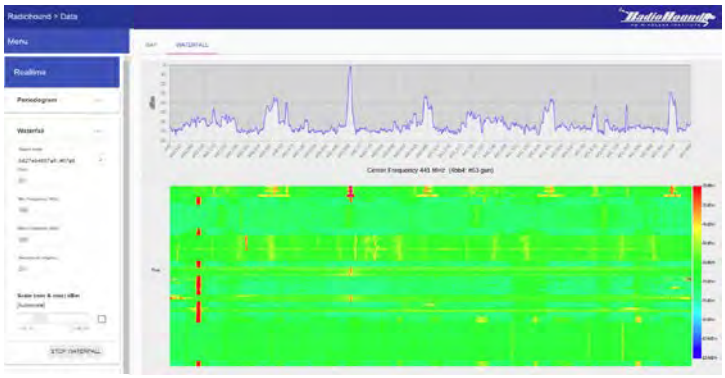
Grad Student or Postdoctoral Mentor: Nikolaus Kleber
Other Contributors: Abbas Termos, and Scott Null

Spectrum mapping is a form of signal processing that creates a visual representation of the presence of a signal across a geographical region. The U.S. Army, Google, and Amazon have use for the graphical data our sensors can provide. Mapping can be used to track walkie talkie usage, or to map which frequencies are being used for Wi-Fi, TV, radio, or personal communication. When computing the spectral density estimation by way of the Fast Fourier transform (FFT), the signal in the time domain transforms to the frequency domain. After transformation, there is an issue with proper scaling of amplitudes to the final graph. To rectify this, I used applied mathematics of the Welch periodogram method to correct for the amplitude.





Programmable and Reconfigurable Millimeter-Wave Circuits and Antennas

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Faculty Advisor: Dr. Jonathan Chisum
Grad Student or Postdoctoral Mentor: David Connelly

As the frequency of distributed microwave circuits corresponds to their physical geometry, there is a need for reconfigurable radios and antennas that operate over a wide range of the electromagnetic spectrum. Currently, advanced RF ICs enable extremely wideband operation, but lack corresponding antennas and other distributed structures. One way to achieve reconfigurability in such distributed structures is with spatial patterning of phase change materials such as vanadium dioxide, or VO_2 — when cold, it is an insulator; when heated, it is a conductor. However, a disadvantage of the material is that the conductivity of VO_2 is 10^5 S/m, two orders of magnitude less than that of most metals, 10^7 S/m, meaning that VO_2 alone dissipates much more energy than metal. The goal of this project is reconfigurable distributed circuits using pixelized metal inclusions on a VO_2 layer with a control mechanism of either spatial UV switching or localized thermal switching.

In preliminary measurements, pure VO_2 CPW transmission lines with metallic launches resulted in extremely lossy lines. In a study of loss and isolation, a coplanar waveguide including unit cells of aluminum and VO_2 was varied in VO_2 thickness, unit-cell gap, CPW cross-section (trace width), and unit-cell size. In the transmission line simulations, aluminum launches were included around the unit-cells, and loss and isolation per unit-cell were extracted. Three different simulators were compared (ADS Momentum, ADS TLIN, and Ansys HFSS) in an attempt to show agreement across software and gain confidence in the model and measured values. Simulation results from parametric sweeps showed ADS Momentum (MoM) and ADS TLIN (Circuit) in close agreement, while HFSS predicts similar trends across frequency but with higher loss. The approach is promising as results show sufficiently low loss for a distributed circuit of length λ, but it requires care in balancing loss and isolation. High-quality VO_2 films at greater thicknesses are necessary, and unit-cell gaps should be small (≤200nm). Loss can be further reduced by trading off programmable resolution by using larger unit-cells. The next steps of this project involve fabricating the lines and comparing real measurements to simulations.

Optically-Controlled Tunable Microwave and Millimeter-Wave Devices for Adaptive Wireless Communications

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This project investigates reconfigurable microwave circuits based on photo-induced electromagnetic band gap (EBG) structures. EBG structures allow the circuit to interact with electromagnetic waves and create stop-bands, pass-bands, and band gaps for wave propagation. EBG structures can be employed for antenna and filter designs and have been researched extensively in the field of wireless communication. The ability to dynamically reconfigure the EBG patterns allows the circuit to be tunable and reconfigurable, and therefore the circuit frequency response can be altered. In this project, the EBG patterns required for reconfigurability can be generated using a novel optical control approach that avoids any complicated fabrication processes. In brief, the approach takes advantage of photo-induced free carriers in a semiconductor, and the EBG patterns can be directly projected onto a Si or Ge wafer to serve as a microstrip transmission line ground plane. By projecting different photo-patterns onto the semiconductor, tunable EBG band-stop filter (BSF) frequency response can be realized. For a prototype demonstration, a tunable/reconfigurable microwave BSF for X band has been designed, simulated, and studied. Both the BSF center frequency and stopband bandwidth can be dynamically tuned. This shows that the proposed approach is promising for the development of tunable/reconfigurable circuits from microwave to the THz band for many practical applications. The research explored in this presentation involves the simulation of components utilizing EBG structures using HFSS (High Frequency Electromagnetic Field Simulation Software); simulations with the optically illuminated EBG on Ge substrates were also investigated. Prototype circuits have been fabricated and assembled for measurements. The knowledge obtained from these simulations along with additional research was used to aid in the development of a new prototype reconfigurable and tunable EBG component.

Passive, Crowd-Sourced WiFi Characterization

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In the technology driven world of today, WiFi is utilized by billions of people across the globe all the time. So, it is crucial that the WiFi is fast and trustworthy, but bad signals and roaming connections create problems for us. How are we supposed to know where to focus our attention to fix the connectivity issues that arise? Our proposed solution is an application that generates a “health assessment” of the WiFi signals in the area.

The application runs in the background to periodically connect to the web and gather network data. With implementations for local and online storage, users may view any data collected in the past as well as data collected by other users. This information is then used to make line graphs and Google maps that display the variations of WiFi strength in a creative way. The program runs as a service, gathering network statistics to address connectivity concerns and in turn help make the world more connected.

An Analysis of Lead in Local Roads, Homes and Historical Industries: How South Bend's History is Poisoning its Children

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Lead is a heavy metal that is absorbed by the bones and brain in much the same way as calcium. However, unlike calcium, lead is toxic. Its effects can be extremely dangerous, especially to young children whose bodies and minds are still growing and developing. Elevated blood lead levels can lead to neurological deficits, behavioral changes, stunted growth, and even decreases in IQ.

In light of these cognitive and physiological deficits, it is important to learn where and why lead hazards are present in any community. When a 2016 report showed that up to 35% of the children had elevated blood lead levels in some areas of South Bend, research was quickly initiated to determine the cause (Figure 1). Causality for lead contamination is usually associated with mining, manufacturing and in exposure to residues of leaded gasoline or paint. While all of these likely play a role in South Bend's lead contamination, it is important to find their relative contributions to exposure risk in order to determine the most effective strategy to mitigate health hazards.

My summer project was to link lead exposure risk to historical activities that generated lead. Previously, other students have collected data about lead exposure from interior and exterior lead paint in homes. I focused on areas where lead hazard from leaded gasoline or industrial activities would be obvious. Soil samples (n=100) were taken alongside South Bend roads as well as at historical sites of battery manufacturers and paint manufacturers. These samples were tested for lead using an x-ray fluorometer and then compared to soil lead levels found at homes and parks. Soil coring was also utilized in an attempt at depth analysis for lead in the soil. However, it was hard to find urban soil that had not been disturbed. The soil lead levels in parks were all less than 40 ppm, and there was a generalized pattern of increasing lead soil levels with proximity to the downtown area, with median levels of 250 ppm. Many sites showed lead levels above the EPA action level of 400 ppm. Knowledge of these findings is important for the continuing remediation process in South Bend.

Development of a Paper-Based Colorimetric Test to Detect Oxytocin

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Oxytocin is a nine-peptide hormone naturally produced by the body. It helps in all stages of a pregnancy as it induces labor, aids in contractions, and helps prevent and treat post-partum hemorrhaging. Injectable oxytocin is one of the drugs listed by the World Health Organization (WHO) as an “essential” medicine.

A 2016 WHO review found that one in four women in Africa who was treated with oxytocin received a substandard shot. For this reason, it is important to develop a cheap, quick method for pharmacists and midwives to test samples without the use of complicated instruments. The problem with developing tests to detect injectable oxytocin is that the concentration of active pharmaceutical ingredient (API) contains only 16.4 ug oxytocin/mL, so it is necessary to produce highly colored products with only a small amount of sample.

This research focused on the detection of the phenol in the tyrosine amino acid present in oxytocin (Figure 1) via Folin-Ciocalteu reagent. Folin-Ciocalteu reagent is a phosphomolybdate and phospotungstate acid that reacts with phenols in alkaline conditions to produce a blue color. Although the Folin-Ciocalteu reagent produced a vivid color change with powdered tyrosine, powdered oxytocin, and injectable bovine oxytocin (which is twice the concentration of human oxytocin), the response was not as strong with human oxytocin.

Steps were taken to optimize the test with human oxytocin. The reaction worked best when the Folin-Ciocalteu reagent was placed down on the paper and allowed to dry and crystallize before the oxytocin was added, followed by sodium hydroxide. Unfortunately, the color change is not sufficiently vibrant compared to water, and the Folin-Ciocalteu reagent is not sufficiently stable when stored on the countertop. To combat this, smaller circles are being tested so that less reagent is used and to concentrate the color change. This research serves as the first steps to develop a method to detect substandard injectable oxytocin in low- and middle-income countries.

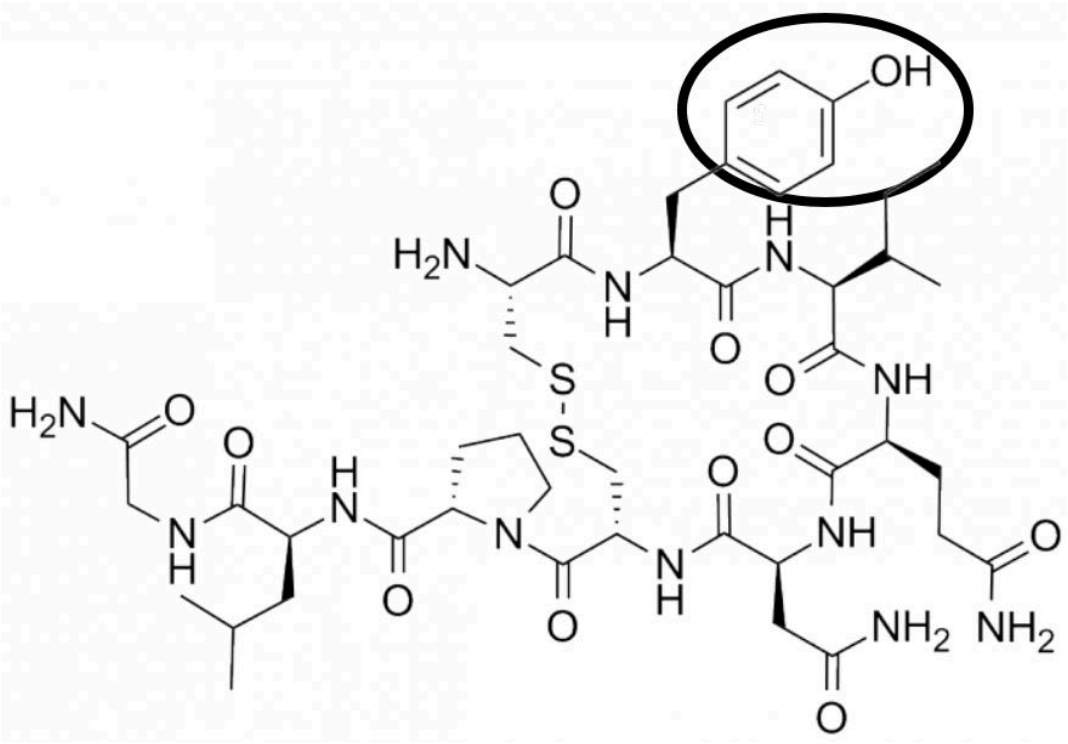

Figure 1. Structure of oxytocin. The phenol in the tyrosine amino acid that reacts with the Folin-Ciocalteu reagent is circled.

Getting High on Science: Surface-Enhanced Raman Spectroscopy for Illicit Drug Detection

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In 2016, over 60,000 people in the United States died from illicit drug overdoses according to the National Institutes of Health, making detection of trace amounts of illicit drugs crucial to law enforcement and public health concerns. Previous studies have shown that surface-enhanced Raman spectroscopy (SERS) is an effective technique for the detection of illicit drugs, but a comprehensive study has never been presented. Since illicit drugs sold on the street are frequently cut with diluents—substances used to dilute drugs—or adulterants—substances added to drug samples to alter their effects—detection of illicit drugs prior to consumption needs to be possible in the presence of such interferents. We aim to use SERS to detect drugs of abuse in samples containing various amounts of common cutting agents. We prepared SERS samples by aggregating silver colloids with various combinations of diethylcarbamazine (DEC)—an opioid simulant—and different interferents. We demonstrate that DEC can be detected using this method even in the presence of high concentrations of interferents. These findings suggest that SERS is a viable method to indicate which illicit drugs are present in confiscated street samples. With sensitive and selective identification of samples, law enforcement can better trace samples to larger suppliers, and medical professionals can improve treatments for overdose patients.

Stay the Course™ Improves Community College Persistence and Completion

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Stay the Course™, designed by Catholic Charities Fort Worth and evaluated by the Wilson Sheehan Lab for Economic Opportunities (LEO), is a program that aims to help community college students of low-income status succeed in their academic careers. Persistence and completion rates in this sector have proven to be significantly low, with nearly 50 percent of students dropping out. Without a college degree, students are likely to face lower earnings and a greater risk of unemployment. Stay the Course™addresses this problem by helping eligible students who show interest in the program solve personal, non-academic, social and institutional problems that might lead them to drop out of college. Through the program, students are paired with a mentor who provides wrap-around case management, and students are also given access to emergency financial assistance. LEO is evaluating the impact of the Stay the Course™ program through a randomized control trial, in which eligible students are randomly selected to receive a spot in the program. Results of the LEO evaluation of Stay the Course™ show that participation in the Stay the Course™ program is positively correlated to higher credit hours attained by the student and a decrease in the likelihood of dropping out of college. These results illustrate the effectiveness of Stay the Course™ in aiding students of low income graduate from college and advocate for the replication of the Stay the Course™ program at other community colleges to improve graduation rates and provide greater opportunity for students of low-income status.

Exhaustive Heterogeneous Graphlet Counting for Network Alignment

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In this project, we develop a new computational method to help scientists compare real-world networks to study aging, disease, public health, and more. A network consists of nodes (e.g., proteins in a biological network or people in a social network) and edges (interactions between the nodes). The goal of network alignment, a popular computational problem in the field of network science, is to map similar regions to each other. In the case of protein-protein interaction networks, a node mapping allows biological knowledge to be transferred from a well-studied species to a less-studied species. Advances in biotechnologies have brought an abundant supply of data in the form of heterogeneous networks, which, by definition, have multiple types of nodes and/or edges. In response, the Complex Networks lab has generalized traditional homogeneous network alignment into novel heterogeneous network alignment, which takes advantage of node type information to generate a more accurate mapping.

Graphlet counting (describing the neighborhood of each node in a network by finding the specific two-to-four-node sub-networks that it belongs to) is typically the first step in network alignment. The current non-exhaustive method for counting heterogeneous graphlets tracks combinations of node types in each graphlet, but loses information by ignoring the node positions at which the colors occur for the sake of reducing computational complexity. In contrast, for this project, we exhaustively account for both combinations and positions of node types, thereby preserving more information about each node's network neighborhood so that it can hopefully be more accurately mapped to a corresponding node in the other network. Next, we plan to evaluate the differences in runtime and accuracy between the exhaustive and non-exhaustive approaches. In addition, we introduce a new (both homogeneous and heterogeneous) graphlet counting algorithm, which is expected to yield some speed-up.

A Web-Based Tool for Flexible Learning-Free Segmentation And Reconstruction for Sparse Neuronal Circuit Tracing

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Similar to how genomics has provided insight into the composition of our DNA, connectomics, the study of the mapping of neuronal circuit tracings, shows potential in explaining how the anatomy of the brain relates to behavior and function. Recent advances in imaging have allowed researchers to generate massive amounts of data in the field of neuroscience. Machine learning-based algorithms provide an effective approach for processing these images into tracings of neuronal circuits. However, learning-based approaches suffer in that training sets require a large amount of ground-truth data that is slow and costly to obtain. The Flexible Learning-Free Reconstruction of Neural Circuits pipeline (FLoRIN) is an alternative approach which utilizes classical, learning-free computer vision methods to perform the automatic segmentation and reconstruction of images of the brain. FLoRIN is a fast and robust pipeline that performs well with the challenge of sparse segmentation without the need for training. Here, we present a web-based tool that makes FLoRIN more accessible to researchers analyzing the connectome. This web-based extension of FLoRIN provides a highly tunable pipeline of computer vision techniques which can be customized to fit an individual's needs. With this web-based tool, researchers are able to perform the segmentation and reconstruction of neuronal circuits directly in a web browser.

Classifying marshland plant species by processing light reflectance in satellite images

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Background - The Random Forest classification algorithm has become very popular in the remote sensing community for its ability to accurately identify such things as forests, bodies of water, urbanized areas, and agricultural plots in satellite images because these surfaces have greatly differing light reflectance bands. However, the remote sensing community has not used the algorithm as commonly for classifying surfaces that slightly differ in their light reflectance bands, like different forms of vegetation. The Smithsonian Environmental Research Center and the McLachlan Lab at Notre Dame are interested in the changing abundances of salt marsh plant species in a research wetland that has been studied for 30 years. A remote sensing reconstruction of such changes within the research wetland would complement controlled experimental work in this area.

Methods and Results - We were curious whether we could differentiate grass species based on small spectrum differences picked up in the Landsat 8 Operational Land Imager (OLI) light reflectance data. Ordinal population abundance data for five different grass species was provided by the research center in order to train the classifier. An added challenge for calibration was that the research center's data are from small vegetation plots making up less than one percent of the remotely surveyed area. As a result, we were able to successfully identify Phragmites, an invasive species in the area, as well as Schoenoplectus Americanus, but with some degree of noise and uncertainty. The Random Forest algorithm did well at averaging multiple ordinal scores found within a 30 meter OLI resolution and was also able to identify when a species was absent from that space with 80 percent accuracy.

Future - We are now investigating whether the classifier can be used on past Landsat 8 images with the same accuracy and also whether seasonality affects the classifiers results. This would allow us to study population change over time within the Smithsonian Environmental Research Center's marshland. While this model provides a great proof-of-concept classifier for identifying grass species based on low-spectrum differences in their light reflectance bands, further work is needed to properly train the classifier and handle the uncertainty found in the ordinal data.

Poster #51

Lobster: Harnessing Opportunistic Clusters with a Workflow Management Tool for CMS Data Analysis

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In an era of increasingly large particle physics data sets, the need for high-throughput computing is ever-increasing. Fortunately, the Notre Dame Center for Research Computing (CRC) can opportunistically access nearly 25,000 cores as made available by local researchers. With Notre Dame's Lobster workflow management tool and an average of 5,000 to 10,000 idle cores at any given time, CMS data can be run on this cluster, making it larger than all Tier 3 and many Tier 2 CMS sites. As technology advances and resources expand, Lobster must evolve to continuously increase efficiency while consistently being able to harness available cores. With a dynamic system such as this one, the value of monitoring tools throughout the many built-in processes is critical. The Collaborative Computing Laboratory at Notre Dame has built such a tool: the Resource Monitor (RM). The RM is powerful instrument that can be incorporated into systems like Lobster to inform users of performance. This project seeks to enhance monitoring of individual task functions and further the development Lobster.

Classifying Aging- and Non-Aging-Related Genes in Dynamic Protein-Protein Interaction (PPI) Networks

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Network science studies relationships between objects, representing each object as a node and a relationship between two nodes as an edge. Examples of real-world networks include technological systems such as the Internet, social systems such as Facebook, or biological systems such as the protein-protein interaction (PPI) network of a species. In particular, we are interested in studying the latter. In a PPI network, nodes represent proteins (gene products) and edges represent bindings between proteins. Specifically, we are interested in studying the human PPI network and changes in its structure and thus cellular functioning with age. This is important, because incidence of serious diseases increases with age. Due to limitations of biotechnologies for PPI data collection, the current PPI network of human is static, as it spans many different biological contexts. So, how to make it context-specific? In our particular application, how to extract a part of the whole network that is specific to a given age, which over all ages would result in a dynamic, aging-related PPI network? This can be done by integrating the static PPI network with dynamic, aging-related gene expression data. Specifically, by doing this, we can assign age-specific weights to nodes or edges and then declare the highest-weighted network regions as active at the given age. The active network regions then correspond to the part of the whole network that is active at the age in question. We use five existing methods for data integration to do this, which results in five corresponding dynamic, aging-related PPI networks of human. First, in each network, we mimic an existing study by: 1) calculating network positions (centralities) of every node at every age, 2) predicting as aging-related gene candidates those nodes whose centralities significantly correlate (i.e., increase or decrease) with age, and 3) validating the resulting predictions by measuring their overlap with the ground-truth aging-related data. The last step aims to determine which data integration approach, i.e., which network, results in the most accurate predictions. Second, because aging-related genes could show other trends besides increasing or decreasing their centralities with age - e.g., their centralities may periodically increase then decrease with age - we evaluate a novel computational strategy that might be able to better distinguish between aging- and non-aging-related genes. Namely, we evaluate whether one of the two gene groups shows higher or lower variation (fluctuation of a node's centrality over time) than the other gene group. Initial results reveal that aging-related genes fluctuate less than non-aging-related genes, which could be the subject of further research because it is counterintuitive. Additionally, aging-related genes

have higher centrality values (averaged over all ages) than non-aging-related genes, which is encouraging, because it matches findings obtained from existing static network analyses of aging.

Using Crowd-Sourced Genealogy to Analyze the Long-Run Effects of Prohibition

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As genealogy increasingly becomes a major interest in the U.S., crowd-sourced genealogical websites like FamilySearch attract millions of users to add their ancestors to a large family tree. Each ancestor has a wiki-style profile where users attach records—like the U.S. censuses and death records—and add life events from these records to the profile. This creates a large-scale dataset with important demographic information and familial connections for every person in the family tree. For this research, we use a subset of approximately 7 million people born in the U.S. between 1885 and 1905. This sample accurately represents the U.S. population on many important factors, such as mortality.

By scraping this wealth of data available on FamilySearch, we can answer long-run economic questions, like the effects of alcohol prohibition laws on childhood outcomes. We primarily examine how the fraction of childhood in a “dry” county—where alcohol is illegal—affects longevity. This contributes to the body of economic and medical literature examining important childhood factors that influence future outcomes. While previous studies of alcohol exposure examine prohibition from state-level laws, we improve causal inference by examining county-level laws, which have greater variation and less measurement error. We find that these dry counties experienced decreased alcohol-related deaths, implying that these laws decreased alcohol consumption. This decreased consumption creates a natural experiment of the effects of alcohol on children. Using a sibling fixed effects model, we find that spending all of childhood in a dry county significantly increased life expectancy by half a year compared to those in wet counties. This effect is larger for men and is driven by higher probabilities of survival to later ages.

Poster #54

Predicting Body Image through Self- Esteem and Social Networks

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There is extensive research linking body image concerns to high social media usage, and a relationship that appears to be strengthening overtime (Fardouly, 2016). There is also research linking body dissatisfaction to peer influence, with one study showing peer weight-related attitudes and behaviors predict body image concerns (Hutchinson, 2005). However, little research has explored how body dissatisfaction could be related to the size of a person's network. This study was conducted to see if there is a connection between body dissatisfaction and an individual's social network. First, we hypothesize that people with larger networks and more extroverted persons (who typically have large networks) will be more satisfied with their bodies. Second, we expect that self-esteem mediates these relationships. This study utilizes data from the NetHealth project at the University of Notre Dame, which focuses on how health-related behaviors, such as sleep and physical activity, are affected by people's social networks. Surveys were conducted to obtain information about their activities, who they interact with, as well as their mental well-being. Multiple linear regressions and correlations were conducted to find relationships between these variables. The results showed that network size and extraversion affect body satisfaction through self- esteem. Extroverts and those with large networks are happier with their bodies because they have higher levels of self-esteem, and high self-esteem is associated with more positive body images. Since body satisfaction is such a big part of today's society, it is important to understand these social and psychological causes so that awareness can be raised, and extreme behaviors can be avoided.

Archiving Workflows Onto Cloud Based Storage

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Scientists use distributed computing to run large scale computations on datasets efficiently. Workflows separate these computations into more manageable pieces, and are represented as directed acyclic graphs. Workflows are made up of files and tasks, where each task is assigned its own input and output files based on dependencies to other tasks. Scientists may not want to run the same tasks twice and it would be just as acceptable to have the output files from instead. Scientists may also want to collaborate with other scientists using a certain workflow configuration. The archive feature allows users to download other user's workflow outputs given certain permissions so they too can analyze the outputs of a certain workflow.

Generation and Matching of Bipartite Graphs

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Graphs can be used to represent a diverse set of phenomena such as protein-protein interactions, social networks, communication networks and generally any set of objects that are linked. Analyzing large-scale graphs acquired from real-world data provides a multitude of challenges for our current computer hardware and software. It is necessary that we explore potential improvements to our architectures, algorithms, networks, and software tools to allow for efficient computing on graphs. This project focuses on implementing and analyzing an algorithm, Hopcroft-Karp, for maximum matching within bipartite graphs. We present a realistic graph generator capable of generating bipartite graphs that exhibit power-law degree distributions. We then utilize the generated graphs for experimental testing of the Hopcroft-Karp algorithm. Scaling results, an explanation of the algorithm itself, and the implementation are discussed. The potential for improving graph algorithms is apparent, and we discuss exploring techniques for parallelism in the future.

Poster #57

knowledge Diffusion in Global Commerce, Investment and Research

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Other Contributors:

Knowledge diffusion is a key component of globalization and international relations. This work focuses on correlations between knowledge diffusion in global commerce, investment and research. Our analysis has been made using data from the Organization for Economic Co-operation and Development (OECD). Our results suggest foreign direct investment (FDI) is a more effective way to diffuse knowledge than trade goods directly. Further, we observe that countries often fall into into one of two major categories: knowledge destination and knowledge source where each category differs in its correlations with knowledge diffusion impacts. A closer study of a select subset of north american countries reinforces our conclusions.

Long-Run Effects of College Openings: Evidence from U.S. Historical Data

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Other Contributors: Professors Jeffrey Denning and Joseph Price (BYU)

The expansion of higher education in the late nineteenth and early twentieth centuries is one of the largest in American history. To what extent did these college openings actually increase local educational attainment and income? This question is difficult to answer because universities are not located at random, making much of the previous research in this area subject to selection issues. We use data on site selection decisions to compare counties where colleges were established to areas that were close runners-up for the site, which are similar to college-building counties along observable dimensions. In order to follow populations over time, we use data from FamilySearch, a large crowd-sourced genealogical website, and the Integrated Public Use Microdata Series (IPUMS) to connect children and young adults in the 1910 census to their respective entries in the 1940 census. This method of record linking provides us with unique identifiers across censuses, allowing us to link a large proportion of the population while minimizing error incurred by name-matching algorithms. We use a fixed-effects model and find that college openings in our sample are associated with an increase in local educational attainment of about a third of a year. This is driven at least in part by an increased likelihood of attaining higher education. Additionally, people who grew up in college-building counties received a wage about 13% higher than their peers in 1940. These results provide further evidence that new colleges help the local population, suggesting high long-run benefits of making college accessible for underserved populations.

Investigating Patterns of the Gut Microbiome in Long-Tailed Macaques

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While the gut microbiome contains thousands of species, only certain taxa are involved in its health and function. Two bacterial phyla, Firmicutes and Bacteroidetes, are predominant members of the gut and have been tied to the host's diet, nutrition, and health. Here we examine these two phyla and their associations with the gut microbiome within wild long-tailed macaques, a species that lives in close association with humans and also shares similar microbiome assemblages as humans. Fecal samples were collected from populations across Singapore, and the prokaryotic microbiome was characterized using 16S sequencing. Richness, stability, community composition, and the Firmicutes-Bacteroidetes (F/B) ratio were calculated at phylum and family level for each sample. The F/B ratio was correlated to microbiome stability at the phylum level only, but it was associated with both the phylum and family-level community compositions. We also tested whether specific families within Firmicutes and Bacteroidetes were linked to this ratio. While the Firmicutes-Bacteroidetes ratio was associated with changes in the relative abundances of families within both phyla, the composition of Bacteroidetes was more strongly impacted, with Flavobacteriaceae linked to a lower ratio and Prevotellacaeae, Bacteroideceae, and Porphyromonadaceae associated with a high ratio. Surprisingly, these results are contrary to previous findings in the literature, and future work will aim to further examine these patterns.

Perovskite Characterization and Degradation

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Perovskite solar cells have emerged in recent years as a potential solar energy technology Here, the degradation of perovskites and the mechanism of electron transfer were studied. Experimental results were compared on conductive titanium dioxide and inert zirconium oxide. The fluorescence of CsPbBr3 was tracked under both ambient and inert atmosphere to elucidate the effect of oxygen on perovskite degradation. X-ray photoelectron spectroscopy was employed to characterize the film composition. By comparing to standard PbO and TiO2 films, the mechanism was confirmed for the conversion of metallic lead to lead oxide upon irradiation. This study is now considered complete, and the research paper is being prepared for publication.

"Use Your Words": The Role of Emotional Security on Interparental Conflict

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The emotional security theory (EST; Davies & Cummings, 1994) has empirically established that a child possesses a higher-order desire for safety within the family and that exposure to interparental conflict may affect such needed security (Davies & Cummings, 1994). During adolescence, the normative tendency to separate—physically and emotionally—from the family is vital for healthy development (Freud, 1958), but oftentimes results in reduced disclosure to parents (Steinberg & Silverberg, 1986). Preserving family communication is essential during adolescence (Barnes & Olson, 1985), as it is the medium through which parents and adolescents re-establish and negotiate their roles and relationships (Lanz, Iafrate, Rosnati, & Scabini, 1999). Thus, this study examined if emotional security would serve as a mediator to explain the relationship between less overt interparental conflict and positive parent-adolescent communication. The variables analyzed in this study were emotional security (Davies, Forman, Rasi, & Stevens, 2002), parent-adolescent communication (Barnes & Olson, 2003), and interparental conflict (Porter & O'Leary, 1980). The participants involved adolescents (N = 225) aged 11 to 17 years of age (M = 13.2, SD = 1.734) and their parents (N = 450), whose ages ranged from 27 to 62 years (M = 42.68, SD = 6.67). After conducting a Baron & Kenny (1986) regression-based approach to analyze the mediation model, the hypothesis was found to be statistically significant. The findings provide significant information about the consequences of interparental conflict on adolescents that can be promulgated among researchers and implemented towards intervention programs.

Keywords: emotional security, parent-adolescent communication, interparental conflict, mediation model

Landscape Effects on the Gut Community of Long-Tailed Macaques

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Within the gut of animals lies a complex community of intestinal symbionts comprised of both eukaryotes (i.e. helminths and protozoa) and prokaryotes (i.e. bacteria and archeabacteria), that engage in ecological interactions determining community composition and stability, taxa abundance and richness, and host health. Environmental factors external to the host are also known to influence intestinal microbial communities. The jury is still out as to whether internal interactions or external environmental factors are more important in determining microbial community assemblages in the gut. Our study sought to gain insight into the external environmental factors that may govern symbiont composition in the guts of long-tailed macaques, Macaca fascicularis. To investigate symbiont diversity and its relationship to landscape variables, 16S and 18S rRNA sequence data were gathered and related to Geographic Information System (GIS) data using dissimilarity matrices. First, Principal Coordinates Analysis (PCoA) of these matrices showed no association between sample site and community composition of prokaryotes and eukaryotes in the gut of macaques. Next, individual habitat characteristics (such as presence of roadways, percent of forest cover, proximity to businesses, etc.) that differed among sites were compiled into linear mixed models to determine each variable's ability to predict overall microbial diversity and the Firmicutes-Bacteroidetes (F/B) ratio, which is known to be an indicator of gut community composition stability and overall health. Results from these models suggest presence of businesses, major roadways, bodies of water, parks, and suburban areas are significant predictors of microbial diversity and variance in F/B ratios. The results of this study suggest gastrointestinal diversity and key bacterial phyla within macaques are strongly influenced by host habitat.

Poster #63

Probing the Mechanism of Osmium Mediated Carbon-Sulfur Bond Cleavage Using Unsymmetrically Substituted Ligand

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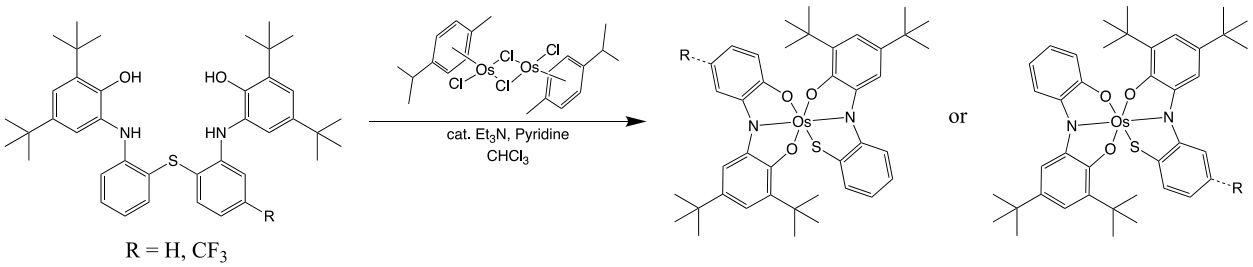
A bis(aminophenol) containing a diphenyl sulfide bridge ($SlopH_4$) reacts with {(*p*-cymene)$OsCl_2$}$_2$ to form Os(ONO')(ONS) via oxygen-carbon bond formation and sulfur-carbon bond cleavage. In this reaction, the aromatic group can either act as an electrophile or a nucleophile to initiate cleavage. To address the question of this mechanism, an unsymmetrical analogue of $SlopH_4$ with a single trifluoromethyl substituent ($FlipH_4$) has been prepared. With lower concentrations of triethylamine and pyridine, the $SlopH_4$ and $FlipH_4$ ligands form dichloride osmium complexes, *cis*-β-(Slop)$OsCl_2$ and *cis*-β-(Flip)$OsCl_2$, with the latter composed of about a 2:1 ratio of isomers. When $FlipH_4$ reacts with {(*p*-cymene)$OsCl_2$}$_2$ and excess triethylamine and pyridine, it forms isomers of CF_3-substituted Os(ONO')(ONS) in a 2:1 ratio. Whether this isomer ratio is dictated by the *cis*-β-(Flip)$OsCl_2$ ratio or by the electrophilicity or nucleophilicity of the aromatic ring will be discussed.



Comparison of Two Dual Spring-Loaded Inverted Pendulum Models of Sloped Walking

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This research aims to compare two models of steady-state bipedal walking at varying ground slopes and speeds. The Dual Spring-Loaded Inverted Pendulum (dual-SLIP) model consists of two massless, springy legs attached to a point mass. In its original passive form, the dual-SLIP model accurately captures the key dynamics of level ground walking. The objective of this research is to determine which actuated extension of the dual-SLIP model best captures the characteristics of slope walking. Two different energy injection/absorption approaches are investigated by manipulating the free length of the leg springs during different phases of gait. In the existing dual-SLIP model A, the free length varies linearly with one slope from touchdown (TD) to mid-stance (MS) and then with a different slope from mid-stance (MS) to lift-off (LO). In the dual-SLIP model B developed in this work, the free length varies linearly with one slope from TD to opposite leg TD and then with a different slope from opposite leg TD to LO. The idea behind this new model is that humans have a better sense of TD events than MS, potentially making the model more consistent with human motor control. The analysis considers ground reaction forces (GRFs) and center of mass (CoM) characteristics over a range of ground slopes to evaluate which model captures more of the characteristics of human slope walking. MATLAB was used to perform a non-linear constrained optimization for a walker with a mass of 80 kg, a nominal leg length of 1 m, and a nominal leg stiffness of 20 kN/m walking at speeds from 1 m/s to 1.6 m/s. Initial results indicate that the GRF and CoM displacements of model A are more similar to experimental human data. Improvements to both models, however, may increase the similarity between the optimization results and experimental human data.

Comprehensive Case Management to Lift Families Out of Poverty

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Despite the prevalence of case management programs throughout the United States, there is little evidence of their impact. Using data from Catholic Charities Fort Worth, we demonstrate the improved labor market outcomes for those receiving treatment. The data used in this analysis comes from Padua Pilot, an intensive case management project for low income families in the Dallas-Fort Worth area. Participants in the Padua Pilot were recruited primarily from Catholic Charities Fort Worth clients who contacted the agency's central intake line seeking a variety of services. In order to be considered eligible for the treatment, clients had to meet the following criteria: reside in Tarrant County, Texas; able to be served in English or Spanish; total family income less than the living wage, as defined by MIT's Living Wage Calculator for Tarrant County; one adult family member between 18 and 55 mentally and physically willing to work; and have not received services from Catholic Charities Fort Worth in the past 30 days. During enrollment periods, eligible clients were invited to participate in the study. Those eligible clients then entered a randomized control trial, creating a treatment group offered comprehensive case management from Padua Pilot, and a control group not offered those services.

Baseline information on participants was compiled prior to randomization from an extensive phone survey conducted by interviewers with the University of Wisconsin Survey Center. Interviewers conducted these surveys approximately 12 and 24 months following the baseline interview. Outcomes of interest in the survey include income, employment status, house situation, debt accumulation, government benefits, and consumption costs. Preliminary results from the intervention offer encouraging evidence on several key outcomes. The results are strongest for the key outcomes Padua Pilot was designed to impact, such as labor market outcomes, but less pronounced results for more downstream outcomes, such as enrollment in social programs or consumption. These results suggest that comprehensive case management does in fact provide assistance to the very families it aims to help.

Influence of Annealing on the Controlled Growth of CsPbBr3 Nanocrystals

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As the energy crisis goes on the need for an alternative energy source is becoming a larger center of research. One of the best sources for renewable clean energy is solar energy, of which we utilize less than 1% of available energy. The current state of the art is Silicon based solar cells, however, CsPbBr3 Perovskites are a cheap and promising up and comer. CsPbBr3 Perovskite's tunable absorption based off of facile anion exchange as well as its low temperature synthesis and variety of manufacturing processes, especially spin coating, makes it a cheap alternative for solar cells. In order to create the bulk films of CsPbBr3 needed for photovoltaic applications, the method of spin coating CsPbBr3 nanocrystals followed by high temperature annealing detailed by Hoffman, et al.,[1] provides a simple synthetic route. As the CsPbBr3 transitions into bulk form, emission intensity and excitonic peak absorption shifts and changes intensity as the nanocrystal leaves its quantum confined state and transitions to the bulk form.[2] This research is focused on measuring the rate of change of the optical and physical properties of CsPbBr3 nanocrystals under high temperature annealing through Photoluminescence measurements and SEM images. Photoluminescence was used to track the change in the emission's peak intensity which is typically reduced by 90% at different temperatures. This change in intensity allowed us to find the peak intensity change and create an Arrhenius plot in order to find the energy of activation of 92kJ/mole for the nanocrystal to bulk growth process. SEM images were used to show the physical change of the particles and quantify the crystal growth over time.

1. CsPbBr3 Solar Cells: Controlled Film Growth through Layer-by-Layer Quantum Dot Deposition
Jacob B. Hoffman, Gary Zaiats, Isaac Wappes, and Prashant V. Kamat, Chemistry of Materials 2017 29 (22), 9767-9774, DOI: 10.1021/acs.chemmater.7b03751

2. Transformation of Sintered CsPbBr3 Nanocrystals to Cubic CsPbI3 and Gradient CsPbBrxI3–x through Halide Exchange, Jacob B. Hoffman, A. Lennart Schleper, and Prashant V. Kamat, Journal of the American Chemical Society 2016 138 (27), 8603-8611, DOI: 10.1021/jacs.6b04661

Designing Energy Efficient Diafiltration Units around Membranes that Separate Molecules of Comparable Size

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In the modern era, increased awareness of environmental health has created a high demand for clean, energy efficient separation processes. Membrane separations provide an attractive alternative to traditional separation methods, by reducing the need for harsh chemical treatments or less efficient thermal processes. For example, after thorough development, the use of membranes for seawater desalination by reverse osmosis can reduce the energy costs by half, compared to equivalent thermal desalination processes. The applications for novel membrane technology in separation processes exist beyond water treatment. With the increasing ability to control membrane properties, such as pore size and charge functionalization, there is the potential to efficiently separate molecules of comparable size.

The main objective of this project can be described as an optimization of diafiltration units with the capacity to separate molecules of similar size. By integrating a transport model of individual diafiltration cells and an overall model of the diafiltration system, the complete model can be optimized to inform the design of energy efficient separation processes. Critically, the predictions of the model must be verified experimentally before its result can be extended. Here, dead end filtration and diafiltration studies on the permeation of potassium chloride (KCl) and magnesium chloride (MgCl2) through NF90 membranes, a commercial membrane with a positive surface charge, are utilized to validate the model. In the filtration experiments, the average ratio of permeate to feed concentrations is 0.0304 ± 0.0032 for a 10 mM MgCl2 solution and 0.1646 ± 0.0642 for a 1 mM KCl solution. In these single salt cases, the salt permeability (B) inferred from these measurements is relatively constant. For the same NF90 membrane, with a mixed salt feed solution of 10 mM MgCl2 and 1 mM KCl, the salt permeability for MgCl2 is approximately the same (0.0490 ± 0.0118); however, as the MgCl2 concentrates in the feed, the salt permeability of the KCl actually increases and the system eventually switches from concentrating

(B < 0) to enriching (B > 0). The solvent flux (Jw) generally increases as the salt concentrates in the feed, because the osmotic pressure increases while the applied pressure remains constant. The hydraulic permeability of the membrane remains relatively constant throughout all cases.

Understanding Lower Critical Solution Temperature Ionic Liquids in the Development of Revolutionary Absorptive Cooling Fluids

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Currently, liquid-vapor equilibria (LVE) is harnessed for a variety of applications, including absorptive cooling systems. However, these LVE conditions result in a large latent heat needed to achieve the phase change from the vapor to liquid state. One way to greatly decrease the energy draw of such ACS systems would be to introduce fluids whose critical temperature is lower than that of standard fluids used in conventional processes, thereby enabling the use of liquid-liquid equilibria (LLE). Ionic liquids, pure salts which are liquid below 100 ˚C, have the potential to function as these lower critical temperature fluids. Typically these low molecular weight salts are readily available either commercially or through fabrication, and often exhibit low toxicity. By understanding and harnessing this technology and switching from LVE to LLE, a significant amount of energy would be conserved to drastically increase the efficiency of these separations.

Investigation of the sorption behavior of organic acids onto catalytic- and food-grade titanium dioxide nanoparticles

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Faculty Advisor: Dr. Kyle Doudrick

Nanoscience and nanotechnology present potential routes towards addressing critical issues such as clean and sustainable energy, environmental protection and human health. Today, nanoscale materials are being used in a variety of different areas such as electronic, biomedical, pharmaceutical, cosmetic, energy, environmental, catalytic and material applications. Consequently, the use of engineered nanoparticles (ENPs) is resulting in increased release of these ENPs into the environment. In order to assess the risk of these ENPs in natural systems, it is required to understand their transport and reactivity. For this, there is a growing interest in studying the behavior of ENPs in aquatic environments. One promising way to achieve this is studying the stability of ENPs in aqueous solutions as a function of pH and ionic strength as well as upon the adsorption of dissolved organic matter.

Among manufactured nanomaterials, titanium dioxide (TiO2) has become widely used because of its chemical and physical properties that can be exploited in different applications including photocatalysts, solar cells, biomaterials, memory devices and environmental catalysts. Consequently, many sources of nanoscale TiO2 could result in the entrance of this material into the environment through air, water or soil. Therefore, the fate, transport, reactivity and risk associated with manufactured TiO2 ENPs released in the environment can be assessed by evaluating TiO2 aggregation in aquatic environments. pH and ionic solutes play crucial roles on aggregation of ENPs in engineered and natural systems. Surface charge titration and EDL screening are two primary ways in which pH and ionic solutes promote NPs aggregation. In addition, naturally occurring organic matter (NOM) in the environment can significantly alter the aggregation behavior of TiO2 ENPs. NOM consists mainly of fulvic and humic substances, which attach to the surface of particles in a variety of ways.

In this study the adsorption of NOM- analogue organic acids (mono-carboxylic acids, di-carboxylic acids, tri-carboxylic acids, and N-carboxylic acids) onto the surface of TiO2 with circumneutral pH and constant ionic strength, is being assessed in order to predict its behavior in natural environments where complex molecules such as humic acid are present.

Batch adsorption experiments were conducted using a group of organic acids with concentrations ranging from 5-100 mg/L, selected to examine a range of structural features in an electrolyte media (10 mM of NaClO4) under circumneutral pH and an

adsorbent concentration of TiO2 of 1 g/L. The organic acids were selected to evaluate the adsorption behavior of particular structures including increasing number of carboxylic acids and phenolic groups.

The outcomes of this project include thermodynamic datasets for Surface Complexation Models (SCM) that will predict the sorption of organic acids onto TiO2 ENPs. These SCMs are useful for studying the fate, transport and bioavailability of ENPs in both aquatic and engineered aquatic systems.

Casting polyvinylidene fluoride (PVDF) using the vapor-induced phase separation (VIPS) method

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Faculty Advisor: Dr. William Phillip
Grad Student or Postdoctoral Mentor: Michael Dugas

Porous membranes are used commonly in several sectors of industry (e.g., water purification and treatment, biopharmaceutical separations and electronics processing). Due to recent research advances, that have led to a better chemical understanding of the membrane fabrication processes, membrane separations offer a path towards a better supply of water for humankind. This poster will focus on the development of membranes for the removal of heavy metal contamination from various sources of water.

Daily human activities, industrial, agricultural, and mining operations as well as the natural presence of heavy metals in the environment make assuring a fresh supply of water for the increasing global population a challenge. In particular, since heavy metal contamination of water supplies poses a threat to public health. One potential approach to address this issue is through the design and development of sustainable treatment technologies such as porous microfiltration membranes with the ability to capture metal ion contaminants.

Microfiltration membranes can be developed through the vapor-induced phase separation (VIPS) methodology. The technique controls the intrusion of water vapor, which is a non-solvent for the polymer, and solvent evaporation to template the polymer membrane with the desired porous microstructure. In the present study, poly(vinylidene difluoride) (PVDF) is used as the matrix polymer due to its ability to partially crystalize into a β-phase, which possess piezoelectric, pyroelectric, and ferroelectric properties due to the atomic orientation within the molecular structure. This particular phase puts a charge in the membrane giving rise to the presence of a strong electrical dipole moment in the monomer unit which is caused by the electronegativity of fluorine. Of particular interest here, these characteristics of the β-phase may facilitate the capture and release of metal ion contaminants. Therefore, it is important to maximize β- phase in PVDF film.

In the present work, the factors that influence the microscopic and macroscopic properties of PVDF membranes fabricated using the VIPS method are identified. In particular, membrane microstructure is controlled by the polar solvent used for the solution preparation, the content of PVDF in the casting solution, and the exposure time in the humid vapor atmosphere. Additionally, the thermal annealing temperature and time influences the β-phase content of the membranes. It is reported that the maximum content of β-phase is achieved at an annealing temperature of 90°C, which in turn increases chain

mobility and thermal energy enough to reorganize the structure. Finally, copolymers additives, such as the mentioned above PMMA-PAA can introduce desired function. The PMMA block can modify the PVDF crystallization behavior and promote the PVDF β-phase crystallization, as demonstrated by the samples with 2% and 3% content. The samples with higher content of poly(methyl methacrylate)-b-poly(acrylic acid) (PMMA-PAA) present a stronger peak in DSC analysis at the characteristic melting temperature of the β-phase which is close to 170°C. PAA segregates to the pore wall during the membrane fabrication to enhance the membrane's ability to capture heavy metals since it promotes a higher charge in the membrane pores. The identification of these processing-properties relationships allows for tailoring of the membrane processing conditions in order to drive towards a successful performance of the membrane.

Elucidating fundamental processing property relationships for chemically patterned membranes

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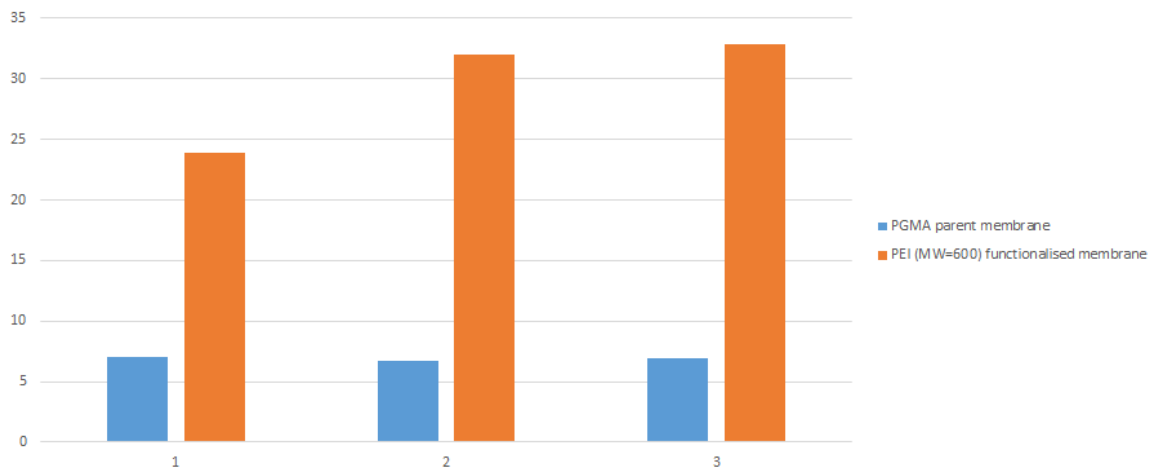
Faculty Advisor: Dr. William Phillip
Grad Student or Postdoctoral Mentor: Feng Gao

Inkjet printing can be utilized to prepare chemically-patterned membranes of different feature sizes and patterns. An example of chemically-patterned membranes is charge mosaic membranes, which have patterns of alternating positively-charged and negatively-charged domains on their surface that traverse the membrane thickness. The arrangement of these domains allows the positive and negative ions to permeate through the membrane faster than neutral molecules of a comparable size, which helps in separating charged species from neutral molecules. The patterns on the membranes can be designed and printed as alternating stripes, squares (cubically-patterned), or triangles (hexagonally-patterned). The feature size of a membrane corresponds to the edge length of each square in case of cubically patterned membrane or the height of the triangle in a hexagonally patterned membrane. The transport experiments, primarily pressure driven filtration experiments, performed using these membranes showed that the concentration of ions was enhanced in the permeate as compared to the filtrate. In these experiments, it was observed that changing the feature size and type of pattern affects the separation performance. For example, a hexagonally-patterned membrane shows higher negative rejection than a cubically-patterned membrane of same feature size. Similarly, a hexagonally-patterned membrane of smaller feature size has better selectivity than that of a mosaic membrane with the same pattern but larger feature size.

In order to improve the selectivity and increase the density of specific ion interactions with the pore walls, the pore wall chemistry was modified. Membrane fabricated using a poly(acrylonitrile-co-oligo(ethylene glycol) methyl ether methacrylate-co-glycidyl methacrylate) (P(AN-co-OEGMA-co-GMA)) copolymer were used as templates because it is amenable to straightforward reaction schemes that decorated the pore walls with specific molecules known to interact with target ions.The modification of pore chemistry is completed in two sequential steps. First, the pore walls lined by epoxide groups were reacted with polyethylenimine (PEI) based on a nucleophilic oxirane ring-opening reaction mechanism. The conversion of the epoxide groups within membranes immersed in solutions of known PEI concentrations for controlled lengths of time was studied using Fourier Transform Infrared Spectroscopy (FTIR). On analysing a series of FTIR spectra between unreacted and reacted membranes, it was concluded that complete conversion occurred with 2M PEI (MW=600 and MW=2000) in 4 hours. The separation performance of the P(AN-co-OEGMA-co-GMA) parent membranes and the PEI-functionalized

membranes were tested using solute rejection experiments. The rejection values for Mg2+ were calculated using PEI-functionalized membranes (PEI with MW=600 and MW=2000) and the P(AN-co-OEGMA-co-GMA) membrane. The results demonstrated that the rejection of magnesium chloride (MgCl2) is around 7% for the PGMA membrane and 30% for the PEI (MW=600) functionalized membrane. These values indicate that the pore walls are charged in the second case which leads to higher rejection values. The second step of the reaction was the carbodiimide coupling reaction of 4-imidazole carboxylic acid to the pore wall. FTIR analysis indicated that a high conversion from PEI-functionalized pore walls to imidazole-functionalized pore walls was achieved through 72 hours reaction using 4-imidazole carboxylic acid. These results show that the surface chemistry of the membranes can be modified to create membranes that allow higher throughput of flowing solutions.



Rejection of magnesium chloride (MgCl2) is around 7% for the PGMA membrane and 30% for the PEI (MW=600) functionalized membrane

Improving Drug Efficacy Through Supramolecular Affinity

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Grad Student or Postdoctoral Mentor: Adam Braegelman, Michael VandenBerg

The use of reversible, non-covalent supramolecular interactions affords routes to materials with tunable function for a variety of applications. Certain host-guest afford high affinity binding for complementary small molecule guest motifs. One such interaction with the N-terminal phenylalanine on insulin was shown to promote enhanced stability, solubility, and efficacy of the protein when a macrocycle was covalently fused to a hydrophilic polymer. To determine the utility of this approach as a platform excipient for the stabilization of many different protein drugs, we have worked to devise assays for real-time monitoring of protein aggregation. Leveraging the change in optical density of a protein upon aggregation, we replicated stressed storage conditions and determined the stability of insulin and related proteins under these conditions. Additionally, we are developing novel synthetic routes to access macrocycles, for exploration of its use in conjugation chemistry. These modified macrocycles will expand the use of supramolecular chemistry to facilitate new drug delivery or drug capture technologies.

Chem. Soc. Rev., 2017,46, 6600-6620

Webber, Matthew J. et al. “Supramolecular PEGylation of Biopharmaceuticals.” Proceedings of the National Academy of Sciences of the United States of America 113.50 (2016): 14189–14194. PMC. Web. 13 July 2018.

Design of Experimentation to Test Faradaic Efficiencies of Plasma-Liquid Systems

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Grad Student or Postdoctoral Mentor: Hernan Delgado
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Plasma electrolysis is an electrochemical process where one of the metal electrodes in an electrolytic cell is replaced by a plasma (or gas discharge). In this configuration, the chemistry is driven by highly reactive dissolved species, such as the solvated electron (e-aq) and the hydroxyl (OH) radical. Plasma electrolysis has significant promise for materials synthesis, water purification, and chemical processing. Using a plasma cathode, our specific focus has been on understanding the inherent limitations to the Faradaic efficiency in a plasma electrolytic cell using two model systems: the classic ferri/ferrocyanide redox couple as well as the dissociative electron attachment to chloroacetate. Using optical absorption spectroscopy and an ion sensitive electrode, the respective concentrations of ferricyanide and chloride can be measured. The main focus of this research has been to measure the Faradaic efficiency of the reduction of ferricyanide under various plasma electrolysis conditions to understand how plasma-generated species affect the Faradaic efficiency at the plasma-liquid interface. The Faradaic efficiency is measured as a function of ferricyanide concentration. Then, various OH radical scavengers such as glycerol and methanol, as well as active stirring, can be introduced to the system to further change the Faradaic efficiency. Due to complexities in the chemistry of ferri/ferrocyanide, such as the backward oxidation reaction, an alternative experiment based on the dissociative electron attachment to chloroacetate is being developed. A stable chloride ion is produced in the reaction of chloroacetate and solvated electrons, which can be measured using an ion selective electrode. This system may help prove that e-aq is the main species responsible for the reduction at the plasma cathode.

Magneto-Electric Silica Nanoparticles (Mag-E-Si-Ns) for Combinatorial Chemotherapeutics Against Metastatic Cancers

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Presently cancer treatment drug formulations involve only one type of drug being administered at a time due to the physical toll on the body. However, treatments have the potential to be much more successful if multiple chemotherapeutics were administered at one time. Additionally, treatments currently kill many non-cancerous cells along with the tumor. The Nallathamby lab has developed Magnetoelectric silica nanoparticles (Mag-E-Si-Ns) loaded with drugs that can be spatially directed to specifically penetrate malignant cells while sparing normal tissues. Combination therapy is very important in achieving more effective results as many cancers are mutating or becoming drug resistant. Additionally, using targeted Mag-E-Si-Ns mitigates the debilitating side-effects of current chemotherapeutic regimens by using the Mag-E-Si-Ns as a nanocarrier for delivering low doses of therapeutics with increased accumulation of the therapeutics at the tumor site through magnetic field guidance.

In this study, we investigated if two or more anticancer drugs encapsulated within a magneto-electric nanoparticle (Mag-E-Si-Ns) could be co-administered as a single dose in an in vitro model system. The four cell lines tested were MDAMB231 (triple negative breast cancer), PC3 (prostate cancer), A2780 (chemoresistant ovarian cancer), and HUVEC (endothelial control cells). The Mag-E-Si-Ns are a drug carrier system, so the chemotherapeutics were magnetically guided directly to the cancer cells by using permanent magnets. Instantaneous release of the encapsulated drug molecules was triggered at the cancer cells site by exploiting the rapid expansion and contraction of Mag-E-Si-Ns in an external electromagnetic field. Once the drugs were released, we observed if they successfully inhibited cancer cell growth and cancer cell migration while avoiding damage to healthy control cells.

Initial results have indicated very effective drug delivery to the cancer cells. There was a dose dependent cytotoxicity specific to cancer cells and not control cell lines. When drug-loaded Mag-E-Si-Ns were administered to the cells and exposed to a permanent magnet and alternating current, the cancer cells reacted with the greatest sensitivity. This was in stark contrast to free drugs that killed all cell types. These results demonstrate that it is possible to selectively deliver chemotherapeutics to cancer cells and release them on demand at dosages lower than current treatments.

Validation of the MicroBio PAD by testing drinking water quality in Nepal.

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Other Contributors: Mary Margaret Green

Water is a basic necessity of life, but many people throughout the world do not have access to clean and safe drinking water. In developing countries, such as Nepal, drinking water comes from a variety of sources, many of them contaminated by coliforms. In an attempt to detect the amount of bacteria present in water sources, a MicroBio PAD was developed that senses Escherichia coli, a common indicator for other harmful bacteria. In this study the MicroBio PAD was compared to two verified but time consuming and expensive tests—the Most Probable Number (MPN) and the ECA Check Easygel. Fifty drinking water samples were collected from Nepal in duplicate and the MicroBio PAD, ECA Check Easygel, and the MPN tests were performed on each sample in resource limited conditions at the Kathmandu Applied Institute of Science (KAIS). The two verified tests, the MPN and the ECA Check Easygel, showed positive results for E. coli 70% of the time. The MicroBio PAD agreed with these two tests 40% of the time. Repeating this study with a similar number of samples in less-limited lab conditions may help determine the cause of this low percentage of agreement. If this future work shows a higher percentage of agreement, the MicroBio PAD may be used independently of the MPN and ECA Check tests to test the quality of drinking water globally, thereby reducing time and costs and making widespread sampling in resource limited settings more viable.

The Development of a Yeast Biosensor for the Detection of Prednisone

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Faculty Advisor: Dr. Don Paetkau

Substandard, spurious, falsely-labelled, falsified, or counterfeit (SSFFC) drugs are a problem worldwide. Ayurvedic medicines can also be falsified by the addition of allopathic pharmaceuticals, such as steroid hormones. Therefore, a cost-effective detection method for the presence of added pharmaceuticals in ayurvedic medications is needed. To address this problem, a Saccharomyces cerevisiae biological sensor was created by adapting an already existing tetracycline responsive promoter/LacZ reporter gene system (AH109::pCM176). The new yeast strains (CML282::pCHAMP18, pCHAMP10 or 11) consisted of a glucocorticoid binding receptor (pCHAMP18), and a glucocorticoid receptor responsive promoter connected to a reporter gene- either LacZ (pCHAMP10) or MEL1 (pCHAMP11). These two plasmid systems were successfully integrated into yeast, fixed onto paper using hydrogel, and shown to effectively respond to prednisone. Both strains were field tested in Nepal during June of 2018 using ayurvedic and allopathic samples. The samples were collected from private, urban pharmacies predominantly in the Kathmandu Valley area. Challenges of working in a resource limited facility are being addressed to provide improvements of the sensor. Discussions with Nepali scientists also suggested additional testing of the ayurvedic samples for microbial and heavy metal contamination should be pursued.

Poster #77

Copper(I) & Copper(II) binding to the ectodomain of human Ctr1

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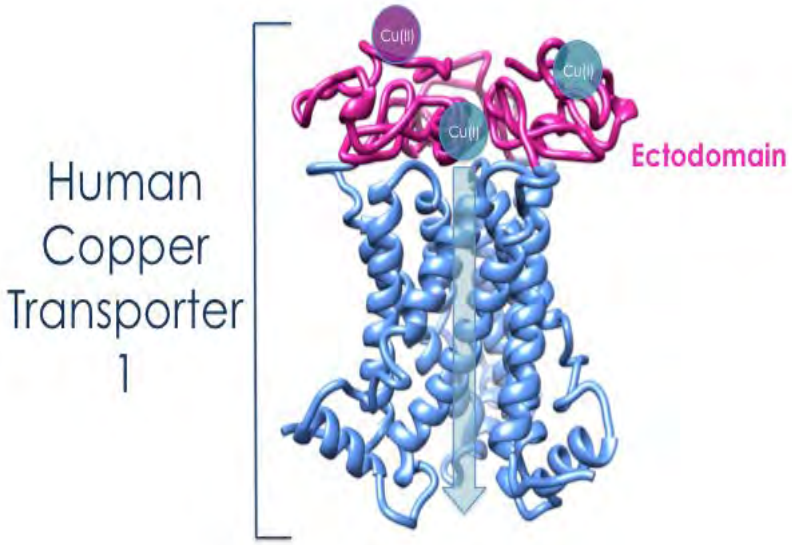
The regulation and transportation of copper in human cells is of utmost importance to avoid reactive oxidative species production and cell death. Cell death can result from oxidative stress, which is a marker for Alzheimer's disease. Human copper transporter 1 (hCtr1) maintains cell vitality by safely transporting copper (Cu) across cell membranes. Model peptides of the hCtr1 ectodomain have displayed interactions with both Cu(I) and Cu(II); however, the stoichiometry of Cu ions to peptide has never been probed until now. Through spectroscopic methods, including UV-Vis and synchrotron radiation, the stoichiometries of Cu(I) and Cu(II) binding to Ctr1-14 and Ctr1-45 were determined. Advanced understanding of the stoichiometry reveals more about the Cu ion binding and transportation abilities of the hCtr1 ectodomain. These abilities can imply how dysfunction of the hCtr1 ectodomain can result in diseases marked by oxidative stress, and thus further research on Cu control and regulation in Alzheimer's disease.



New nanocapsules for drug delivery

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Faculty Advisor: Dr. Bradley Smith
Grad Student or Postdoctoral Mentor: Sasha Padilla

Nano-carriers have become a popular method for treating cancer since these are efficient at delivering dyes, nutrients and drugs to specific tumors. These structures range from 1–1000 nm in diameter and they made of a wide variety of materials (e.g. polymers, lipids, carbon tubes, dendrimers). Our approach to treat malignant tumors utilizing drug loaded liposomes and polymers. Liposomes are effective nano-capsules that have been in use since the 1960's. These structures are composed of at least one phospholipid bilayer, and previous research has shown that liposomes are useful for delivering drugs, dyes, nutrients and other compounds. Moreover, in this research we assemble Large Unilamellar Vesicles (LUV) composed of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) and 1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-L-serine (POPS). We use different proportions of these lipids while verifying their stability and content release. After preliminary studies with liposomes, a subsequent goal of this project was to determine if fluorescent ZnDPA probes, specifically PSVue 380, will show weak interactions with the core of a nano-particle synthesized by the Gao group. This novel hyperbranched polytriazole polymer displays a core shell architecture that possess a polycarboxylate center. The probes show enhanced florescence when they interact with an anionic surface (e.g. liposomes or dead / dying cells) suggesting that the nano-capsule polymers can bind cationic drugs in their core. We hypothesize that high drug loadings can be achieved with these new nano-capsules.

Computation Spectroscopic Analysis of Alpha Amyloids of PSMα3

Olanrewaju Olafuyi
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College of Science

Faculty Advisor: Dr. Arnaldo Serrano
Grad Student or Postdoctoral Mentor: Dean Edun

Phenol-Soluble Modulin (PSMα3) are virulence factors secreted by staphylococci aureus. PSMα3 is known to stimulate the inflammatory responses as well as the destruction of human cells due to the formation of the cross-α amyloid fibrils. While most Eukaryotic amyloids are known for their cross-β strands in which runs perpendicular to the fibril axis however, this specific amyloid has a unique α-helical- structure. Using previously determined crystal structures, computational spectroscopic simulations were performed in order to identify possible signatures of these novel structures in the Fourier Transform Infrared (FTIR) and Two-Dimensional Infrared (2DIR) spectra. Considerable changes in the spectra upon formation of fibrils are predicted to occur due to coupling of the amide modes along the helical and fibril axes, suggesting a new method for identifying other peptides and proteins that can adopt this unique structure.

Poster #80

Does Cultural Conflict Affect educational Attainment?

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This research examines how community attributes impact levels of college attainment in United States counties. The focal point of this study aims to investigate how perceptions of higher education can form amongst members in communities in the face of cultural conflict. Institutions of higher education contribute to the dominant societal norms and reflect values that may dispute those of conservative Americans. I exploit data representing votes on ballot initiatives in 30 states that sought to ban, from 1999 to 2008, that sought to ban same-sex marriage. Utilizing this data, I examine relationships between voting patterns on this controversial issue and ensuing levels of educational attainment. Prior research has shown that people with higher-levels of education show greater support for same-sex marriage, while those with lower-levels of education tend to oppose same-sex marriage. However, little research has examined how views of same-sex marriage impact rates of educational attainment. Despite the importance education has in shaping Americans' future lives, people vary in terms of the value they place on educational attainment. Preliminary findings show levels of academic attainment in the U.S. counties differ based off past voting outcomes. Counties that were highly opposed to same-sex marriage show the smallest growth rates in educational attainment. These numbers hold true even when controlling for previous levels of educational attainment and several other control variables.

Reproductive Health Fears Present in Nahua Indigenous Women: An Analysis of Interactions with Biomedical Personnel

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Maternal and reproductive health in Mexico has undergone changes over the past couple of decades in the transition from traditional midwifery practices to biomedical obstetrics and gynecological care. The Mexican government has created programs, such as Oportunidades, to improve reproductive health within indigenous populations at a localized level. This study was based on participant observation and interviews conducted between 2004 and 2007 on the perception of Nahua indigenous women, clinicians, and midwives on reproductive health in northern Veracruz, Mexico. Our data show that there are several factors, such as local concepts about the body, machismo, and patronizing attitudes from health care providers, which unceasingly foster feelings of unease towards receiving biomedical treatment in the moment of delivery. The manner used to describe the physical effects and risks of contraceptive methods and bilateral tubal ligation are conducive to feelings of distrust towards their local medical community. Fears produced by these factors thwart Mexico's efforts to provide quality reproductive health experiences for Nahua indigenous women. With fewer women seeking out the attention of midwives as their primary source of reproductive knowledge and care, local medical personnel are entrusted to carry quality patient care and implementation of social programs in a population that has been historically marginalized and underserved. The results of this study aim to shed light on how indigenous women manage the feelings of fear and angst brought on by their interactions with biomedical personnel that ultimately hinder an already disempowered community from attaining their ideal state of reproductive wellness.

Machinery Sensing: Analysis and Optimization

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Faculty Advisor: Dr. Thomas Pratt
Other Contributors: Rob Kossler, Eric Jesse

For companies that rely on machinery, equipment health monitoring and system characterization are important to ensure reliable and safe operation. Researchers involved in the Turbomachinery Sensing project are investigating practical methods for achieving these objectives using radio-frequency (RF) non-contact sensors. The team is specifically evaluating RF transceivers to detect vibrations, debris ingestion, and foreign object damage within gas turbines, as well as anomalous behaviors of other machinery. The potential to monitor machines and to detect and diagnose problems will allow companies to develop efficient maintenance plans, save money, and in some cases, save lives.

My specific role in this project was to help in the collection of sensor data in an industrial plant, to expand existing/create new processing applications in MATLAB, to analyze plots generated from test data, and to install and utilize a software design tool known as FEKO to create models enabling the optimization of antenna design and antenna placement. I participated in tests conducted at I/N Tek, a local steel plant. Here, we collected data to characterize vibrations from a rotating drum flanked with gearboxes and data from a “pickling” machine that uses acid to remove rust from steel sheets. Through my analysis of these data, I confirmed in initial analyses that the RF sensors were able to detect patterns in the reflected RF signals that correlated with machinery operation. Finally, to initiate an analysis of sensor application to gas turbine engines, FEKO software tools are being utilized to aid in the development of antenna designs and antenna locations in gas turbine engines. The data products from my analyses and the processing applications I helped to install and operate will be leveraged in the Turbomachinery Sensing project, as Dr. Thomas Pratt and his team continue to work towards the creation of a reliable vibration sensing tool.

Tracking multiple targets using Dual-Polarized Antennas with Software Defined Radios

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Typical radar systems are single polarization systems with corresponding single channel transmitter and receiver operation. The recent advent of relatively inexpensive Software Defined Radios (SDR) facilitates research using multiple channel systems, including systems with dual-polarized antennas and/or spatially separated antennas. The objective of this project was to assemble three dual-polarized radar nodes incorporating a new SDR model (Ettus N310). The work involved hardware integration and software and firmware development to enable control with SDR graphical user interfaces. One radar node has been fully assembled and tested and the remaining two radar nodes will be completed once the remaining components are delivered. Continuous data streaming from the on-board field programmable gate array (FPGA) has been implemented on two of the four transmit channels in the SDR with plans to add this feature to all four channels. The process for verifying the transmit RF power output on each individual channel was also automated using a MATLAB script to take automated power level reading and plot them in a graph for all four channels. The results of this test showed that the SDR transmit power output with UHD Driver release version 3.11 operated correctly but, did not operate correctly with the newer 3.12 version. More work is needed to integrate the SDR with the newer driver version.

Integrated Task and Motion Planning for Robotic Systems

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Intelligent physical systems capable of interpreting, planning, and executing high-level tasks requires reasoning over discrete actions and continuous motions, and that poses unique computational challenges. A recent trend in solving these challenges is integrated task and motion planning (ITMP), which proposes to synthesize both discrete task plans and continuous motion trajectories for mobile robots simultaneously. Successful intelligent autonomous robots are able to perform ITMP in uncertain environments, and that requires the ability to observe and act upon its environment to develop a plan towards accomplishing some task.

Our basic idea is to use a camera for perception and integrating perception in mission and motion planning. This REU project is mainly about developing a demonstration in unmanned ground vehicle robots by combining perception and learning models with ITMP. We aim to develop a control system in which a robot receives a high-level specification on the continuous robot and object state spaces, but with unreliable priori knowledge.

For object detection, we simply used color to identify an object, and we used OpenCV camera calibration and 3D reconstruction packages to gain the intrinsic values of the camera and estimate the real-world location of an object based on images of a single camera. We used a feedback control system for the robot and implemented Robot Operating System with the robot's own control library. For our next step, we plan on integrating perception and control to gradually increase uncertainty of the object's location by giving unreliable locations of the object to the robot and later obstructing it from the robot's initial view. This would evolve to having the robot plan and take actions to find more information about the object it is tasked to find.

Using Augmented Reality to Control a Six-Axis Robot Arm

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Augmented reality headsets offer a suite of hardware and software tools conducive to real-time, user-friendly manipulation of virtual 3D objects located in persistent locations around the user. This research sought to apply these tools to the programming and control of a six-axis universal robotic arm, providing the ability to either control the arm in real-time or to pre-program a sequence of steps to be performed on command. Using augmented reality to provide input allows users to control the arm with a reasonable degree of precision without need for extensive technical training. The application utilizes the orientation of the user's head along with certain recognized hand gestures to allow selection, translation, and rotation of virtual objects. The user controls the robotic arm by manipulating a 3D "cursor" object, which represents the desired location and orientation of the end of the robotic arm. This information is translated into UR Script commands and sent to the robot via network connection, either as the user moves the cursor or in recorded batches. Due to logistical difficulties concerning the availability of the robotic arm, no concrete results are available at the time of this writing, but test users were able to effectively utilize the user interface after only a few minutes of instruction.

Wireless Communications Interface and Services for Drone Swarms

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One of the things that makes drones so popular is that a user can communicate with the drone remotely. These communications send information, such as position or battery level, and commands, which instruct the drone in its movements. Drones become dependent on these communications in order to maintain a safe environment for use. By adding an onboard computing and wireless platform to the drone, we hope to advance and expand upon the communication framework available to the drone. This will include several wireless interfaces. A 4G LTE cellular connection will be established for the drone to communicate to the cloud and ultimately establish drone-to-ground communications. Alongside that, an infrastructure less WiFi network is configured on the computer for drone-to-drone communications. The onboard computer also acts as a communications manager for the drone's wireless interfaces. This allows the drone to monitor the strength of each wireless network and controls the messages broadcast on each. These interfaces and the data we collect from them will allow us to better operate drone swarms and begin implementation of detect-avoid protocols. My goal for this project is to configure an onboard Raspberry Pi 3 B embedded computer in cohesion with an Ad-Hoc WiFi network and a 4G LTE cellular USB modem. This will be the foundation of the message and stream architecture that will be placed on top of the drone. As of now, the Ad-Hoc WiFi connection is operational. Several 4G LTE USB modems from Verizon are being configured to provide 4G LTE cellular service to the Raspberry Pi. By the end of the Summer, we aim to have the full wireless platform running harmoniously and sending data packets between drones using the communications described as above. We aim to conduct tests of the network to examine the strength, speed, range, and other parameters to each medium of communication.

Human-Robot Collaboration

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Robots are expected to work alongside humans in a safe, intelligent, and friendly manner in warehouses, homes, and other robot assistant applications. A key component of such a robotic system is the ability to interpret human intention and operate with knowledge of the surrounding environment. As much of human intention is conveyed through movement, we use a Bayesian non-parametric learning approach to create a human model from motion data. Unlike most human modeling methods, which assume that the number of states is defined, our more flexible method identifies the number of human states directly from the data. We also enable intelligent robotic manipulation of the environment with object classification and localization information generated by a Faster Region-based Convolutional Neural Network. In order to achieve goal-oriented human-robot collaboration and optimize overall task performance, we model sequential tasks as Markov Decision Processes. We demonstrate the effectiveness of our framework in a chair assembly task.

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