Amherst College Summer Research Abstract Book 2023


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Abstract Book Team

Editors
Daniel Oo ‘24, Ashley Bao ‘26, Hasun Noh ‘25, Siri Palreddy ‘24

Cover Art
Nina Aagaard ‘26

Administrative Director of the Science Center
Jess Martin

This booklet showcases the research that Amherst College students have accomplished in the summer of 2023. We hope it serves as a resource for future students interested in undergraduate science research.

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Investigating the Stability and Enzymatic Activity of Mutations at a Disease-Associated Site on Protein Tyrosine Phosphatase 1B (PTP1B)

Sydney Bluestein[1], Anthony Bishop[1]

[1]Department of Biochemistry and Biophysics, Amherst College, Amherst, MA, USA

Introduction: Protein tyrosine phosphatases (PTPs) catalyze the removal of phosphate groups from phosphotyrosine residues. Disruption of regular phosphorylation pathways has been connected to numerous life-threatening medical conditions. Protein Tyrosine Phosphatase 1B (PTP1B) is a well-studied PTP whose misregulation has been associated with human disease. There have been efforts to create effective inhibitors that modulate irregular PTP1B activity, hopefully mitigating disease symptoms. Mutations at arginine 56 in PTP1B along with the arginine at corresponding positions in other PTPs, namely SHP2 and PTPRN, are associated with diseased states such as Hodgkin Lymphoma and Acute Myelogenous Leukemia.

Methods: Site-directed mutagenesis was performed on PTP1B to yield four distinct mutants that correspond to human diseased states. The resulting R56W, R56G, R56P, and R56H mutants were expressed from E. coli and purified. Little information was known about how these mutations would impact PTP1B stability and activity. SDS-PAGE gel electrophoresis was run to access protein purity. Activity assays were performed, comparing wildtype and mutant PTP1B catalytic efficiency. If there were detectable mutant activity, a Michaelis-Menten kinetics assay was run.

Results: The concentrations of the PTP1B mutants were extremely low, and SDS-PAGE results confirmed that these mutations did not express well as they were prone to proteolysis. Activity assay results demonstrated that R56G was the only mutant with detectable activity. R56G's catalytic efficiency was severely reduced compared to wildtype, characterized by its high Km value and corresponding low kcat value.

Conclusion: The arginine at site 56 is vital to PTP1B stability and enzymatic activity, and proteins with deviations from arginine at this site are not viable. Our results provide a biochemical rationale for the connection between mutations at position 56 and human disease.

Selective Allosteric Inhibition of Striatal Enriched Protein Tyrosine Phosphatase (STEP)

Sujit Chepuri[1], Sean Kim[1], Anthony Bishop[1]

[1]Department of Biochemistry and Biophysics, Amherst College, Amherst, MA, USA

Introduction: Protein tyrosine phosphatases (PTPs) are a class of enzymes important to many mechanisms of cell signaling because they catalyze the removal of a phosphate from phosphotyrosines. PTPs are considered important drug targets because when they are misregulated, cancer and many autoimmune diseases can follow. Striatal enriched protein tyrosine phosphatase (STEP) is a brain specific PTP and is part of the kinase interaction motif (KIM) family of PTPs. Overactivation of STEP is implicated in many neurodegenerative diseases including Alzheimer's disease, Parkinson's disease, schizophrenia, epileptogenesis, and Fragile X Syndrome. Therefore, STEP is an intriguing drug target because finding inhibitors of STEP could lead to the development of effective drugs. Most PTPs share a highly conserved catalytic domain near the active site, so active site inhibitors are often not specific to just one PTP. Therefore, allosteric inhibitors that attach away from the active site in a non-conserved region are considered more promising than active site inhibitors for therapeutic inhibition because they can provide more selective inhibition to a single PTP.

Methods: Through crystallographic data found by collaborators in the Daniel Keedy Lab at the CUNY Advanced Science Research Center, it became apparent that two inhibitors, Inhibitor I and Inhibitor III, can bind to two potential allosteric cysteine residues on STEP: C505 and C518. Through biochemical assays performed with STEP and DiFMUP, we aimed to test the potency, time-dependence, selectivity of these inhibitors to STEP, and to determine if C505 or C518 is an allosteric site. After site-directed mutagenesis, we purified 3 STEP mutants from E. Coli; C505S, C518S, and C505S C518S. These STEP mutants were utilized in our biochemical assays testing the selectivity of the inhibitors to

Results: We were able to confirm that Inhibitors I and III were selective to STEP over other classical PTPs. HePTP also showed significant inhibition, which makes sense given that STEP and HePTP are highly conserved as they are both a part of the KIM family of PTPs. As for time-dependence, it appears Inhibitor I binds and inhibits STEP in under a minute, which is extremely fast relative to other PTP inhibitors. We were unable to determine with confidence if C505 or C518 was an allosteric site. It seems as though both sites were able to exhibit some control over the enzyme, as all of the mutants exhibited higher resistance to inhibition relative to wild-type STEP, but the data was not definitive.

Conclusion: Further exploration of the molecular basis of the selectivity of Inhibitor I and III could pave the way for the development of more potent inhibitors as potential STEP-directed therapeutics.

Deep Graph Learning Benchmark for Ligand-based Drug Discovery

Ha Dong[1], Jens Meiler[2, 3], Pia Walter[3], Abdullah Mamun[2], Lily Gao[4], Yunchao "Lance" Liu[2]

[1]Amherst College, MA, USA
[2]Vanderbilt University, TN, USA
[3]Institute for Drug Discovery, Leipzig University Medical School, Germany
[4]Georgia Tech University, GA, USA

Introduction: Drug discovery is an expensive and time-consuming process, often taking 10-17 years and $1-2 billion dollars to develop a single new drug. In early-stage drug discovery, virtual screening, through computational prediction of lead candidates, presents a solution for these constraints. As a powerful deep learning algorithm, graph neural networks (GNNs) can potentially improve the current virtual screening pipeline, given its expressive power in molecular structure. However, due to the lack of standardized datasets, many nascent algorithms are being evaluated on erroneously curated data, making it challenging to gauge method performance. Inconsistencies in evaluation metrics and data splitting further impede the assessment of graph-based QSAR methods. To address these challenges, we present a diverse and high-quality open-source benchmark database and use it to evaluate state-of-the-art GNN architectures, serving as an evaluation ground for the AI drug discovery community.

Methods: The benchmark leveraged multiple high-throughput screening bioassays from the PubChem database. Raw chemical data were hierarchically curated and sanitized by Corina Classic, RDKit, and BioChemical Library to ensure data integrity and reduce false positives. The resulting quality datasets were used to benchmark state-of-the-art GNN architectures, including G2GNN (Graph of Graphs), HiGNN (Inter-Message Passing), MolKGNN, SphereNet, SchNet, DimeNet++ (Chirality-aware), and MVGRL (Contrastive Learning). An open-source benchmark library is being developed with a variety of metrics, data splitting, and graph augmentation methods.

Results: We curated 73 high-throughput screenings that targeted distinct small molecule protein classes, including GPCRs, nuclear receptors, kinases, transporters, etc. Over 20,000 organometallics, mixtures, redundancies, and artifacts were excluded, resulting in a collection of 374,000 quality compounds. Our benchmark offers a data-loading system, evaluation criteria, and tools for graph augmentation, pre-training, and hyperparameter optimization, showing an improved performance across multiple GNN designs.

Conclusion: Our study emphasizes the importance of a consistent curation pipeline and provides an open-source benchmark library to facilitate the development of graph-based QSAR methods. By thoroughly evaluating GNN architectures, we offer a robust comparison between different model designs and how they can address limitations in molecular data such as heterogeneity and class imbalance. Moving forward, we aim to expand the property coverage of the benchmark to further advance AI techniques for drug discovery.

Computational Hydropathy Analysis of BamA mutants on PARCH Scale

Connor G. Farquhar[1], Shivangi Nangia[2]

[1]Department of Biology, Amherst College, Amherst, MA, USA
[2]Department of Chemistry, University of Hartford, West Hartford, CT, USA

Introduction: This research aims to use the Parch hydropathy scale to corroborate previous studies on ecBamA. Examining fatal mutants in the E. coli membrane protein BamA, we aim to display the applicability of chemical analysis in understanding bacterial phenotypes and protein stability. Moreover, the role of extracellular loop six (L6) will be observed and compared to BamA as a whole.

Methods: This experimental study will use computational techniques and analysis to mutagenize and study BamA mutants. After being created in PyMol and placed in a membrane using CHARMM GUI, the mutants will be run through Gromacs and Anton2 for further stabilization. The stabilized systems will then be measured via the PARCH scale, and the resultant data plotted in Excel

Results: The results of this study indicate significant correlation between PARCH values and mutation region. While average PARCH value varied between proteins, it was generally ~.3, indicating a “medium” hydropathy. Moreover, BamA is defined by a highly hydrophobic interior and hydrophilic poles. In every protein, the average PARCH value change was greater than 120%, excluding L6. As with the entire protein, L6 has an average PARCH value in the “medium” range at ~.4, and is composed of both hydrophilic and hydrophobic sectionsFocusing on L6, we found that not only does L6 consistently have higher parch values, but also experienced the largest change in both absolute and percentage change. This trend was seen even outside the non conserved region of L6, impling that these findings are applicable outside of E. coli. The neighboring amino acids were variable: while some mutants showed large changes (particularly the L6 deletions) most showed little to no appreciable results. Directionally, the non-L6 mutant residues (excluding the salt bridge) decreased from wild type, while the L6-mutants and 740 bridge increased. Overall, the results showed a strong correlation between PARCH values and mutation location. Considering that all of the mutants studied presented with low-growth phenotypes, PARCH may be a useful test in determining mutant outcomes.

Conclusion: Through this research, we successfully used PARCH to display the impact of mutations on BamA. Moreover, we were able to support the earlier finding that in E. coli, L6 plays a crucial role in protein stability and that it is prone to large changes in conformation. We also showed that mutation of the 661-740 salt bridge leads to similarly large changes in PARCH measurements. However, we were unable to conclusively determine a correlation between mutated residues and the PARCH values of their neighbors. Nevertheless, these findings suggest that the PARCH scale is a useful tool in protein analytics.

Protamine revives DNA Origami

Shreya Hegde[1], Oliver Polachini[1], Alejandra Velasquez[1], Moumita Dasgupta[1], and Ashley R. Carter[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: DNA origami is used in nanoengineering to build nanostructures for drug delivery or enzyme immobilization. In DNA origami, a single molecule of DNA is folded multiple times to create the structure, just as paper is folded multiple times to create a structure in origami. One issue with DNA origami is that the structures degrade over time. To try to address this issue, we wanted to see if protamine proteins might stabilize DNA origami. Protamine is a protein found in sperm cells that bends, folds, and stabilizes the DNA in the nucleus.

Methods: We made a solution of 0.5 ng/uL of DNA origami rods degraded over five years and 1 mM magnesium-acetate. For slides with protamine, we add 10 uM protamine. We transfer this sample onto the mica slides. We then image the structures on the slide using atomic force microscopy (AFM).

Results: Before the degradation, the rods were about 5 nm tall and 225 nm long. But after degradation, the rods appear disintegrated and unfolded. The height of the DNA rods varied greatly along their length and was, on average, about 1 nm. When we add protamine, we miraculously see folded rod structures with the original dimensions as before. The height mostly remains constant along their length and has increased to about 5 nm.

Conclusion: This data suggest that protamine might be a useful stabilizing agent for DNA origami. Future work would be needed to ensure that these effects are universal over other DNA origami structures and that protamine would not affect the uses of the structures in nanoengineering applications.

Folding dynamics of histone replacement by protamine

Rebekah Hong[1], Isabel P. Hardy[1], Lynn Fu[1], and Ashley R. Carter[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: Understanding how DNA folds in germline cells (i.e. sperm cells) is crucial to studying how epigenetic traits are passed down from parent to offspring. In sperm cells, most histones, which carry the information for epigenetic traits, are replaced by a small positively charged protein called protamine. We are interested in studying this histone replacement pathway. There are two potential models for direct replacement of histones by protamine: 1) screening and 2) active displacement. In "screening," protamine, which is positively charged, increases the positive charge around the negatively charged DNA, causing the histone protein to fall off. Subsequently, the protamine proteins bind and fold the DNA. In "active displacement," protamines directly bind and fold the DNA, causing a conformational change that knocks the histone off. To distinguish between these models, we will look for a DNA unfolding event in the histone replacement pathway.

Methods: We use a real-time folding assay, tethered particle motion (TPM), to measure the folding pathway. In TPM, we tether a particle to a surface using DNA and measure the motion of the particle. If the DNA folds, then the motion of the tethered particle decreases.

Results: Previous TPM data taken at 5 Hz found that the motion of the particle drastically decreased upon addition of protamine, indicating that there was no unfolding step in the histone replacement pathway. This supports the "active displacement" model.

Conclusion: Here, we will present work toward taking TPM data at a faster rate (45 Hz) to determine whether there are any unfolding steps in the pathway that the previous data missed.

Using protamine to aggregate DNA origami rods

Oliver Polachini[1], Shreya Hedge[1], Alejandra Velasquez[1], and Ashley R. Carter[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: In origami, a single sheet of paper is folded multiple times to create many different structures. Similarly, in DNA origami, a single strand of DNA is folded by single-stranded DNA "staples" multiple times to form many different nanostructures. These nanostructures are useful in nanoengineering or drug delivery applications. In this study, we look at how DNA origami is folded by proteins to see if we can find a way to make DNA origami aggregate into supramolecular structures. The protein we are interested in testing is protamine. Protamine condenses DNA in sperm nuclei by creating many DNA-DNA interactions, which might be useful for aggregation.

Methods: We test this protein on DNA origami rods that are 225 nm in length and 14 nm in diameter. To look for DNA aggregates, we measure structures using an Atomic Force Microscope (AFM).

Results: We image DNA origami rods in the presence of 20-200 uM protamine, and find aggregates of several rods together end-on-end or side-by-side.

Conclusion: This process might be useful in creating supramolecular structures for multiple applications in nanoengineering.

DNA folding by Sars-CoV-2 nucleocapsid protein

Jonathan M. Xing[1], Youna J. Choi[1], and Ashley R. Carter[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: Nucleic acids are tightly packaged within a virus before injection into a host cell. Understanding viral packaging could inform the development of more potent antiviral medications and further basic research into the viral life cycle. Packaging in Sars-CoV-2 is done by the nucleocapsid protein (N-protein). N-protein interacts with single-stranded RNA using three binding motifs: specific interactions with a coding region of RNA called the packaging signal, nonspecific interactions with the RNA, and nonspecific interactions with other N-proteins. We are interested in studying nonspecific interactions with RNA that might be occurring between the positively charged N-protein and the negatively charged nucleic acid backbone.

Methods: To facilitate this study, we look at how N-protein interacts with double-stranded DNA which has the phosphate backbone, but not the RNA coding region or any RNA structural characteristics. Here we discuss the creation of the DNA using polymerase chain reaction (PCR) and purification techniques. After creating the DNA, we imaged samples of DNA with and without Sars-CoV-2 N-protein.

Results: We see binding of the DNA by the N-protein and will present results toward measuring the folding interaction.

Conclusion: These studies suggest that packaging within viruses includes nonspecific, electrostatic interactions between the N-protein and the phosphate backbone of the nucleic acid. These interactions are likely to be common to all viruses and might be interesting targets for antivirals.

Perturbation in the extracellular matrix induces the mitochondrial unfolded protein response

Annika Bajaj[1], Avijit Mallik[1], and Cole Haynes[1]

[1]Department of Molecular, Cell and Cancer Biology, UMass Chan Medical School

Introduction: The mitochondrial unfolded protein response (UPRmt) is the mitochondrial defense against misfolded proteins accumulating within the organelle. Given that age-associated diseases like Alzheimer's and Parkinson's are associated with the accumulation of misfolded protein aggregates in the extracellular space, we hypothesized that there might be a similar signaling pathway to the UPRmt that maintains extracellular protein environment.

Methods: hsp-6::GFP crosses (reporter gene), lifespan assays, egg-laying assays, and TMRE staining of mitochondria were conducted on N2 (wild type) and col-179 knockout strains of C. elegans.

Results: No difference in lifespan or egg-laying was observed between control and knockout strains, and TMRE imaging showed no visible difference in mitochondrial quality, indicating knockouts had no detriment to survival or mitochondrial function. However, knockouts for col-179 did demonstrate increased hsp-6 levels, suggesting a higher level of UPRmt activation.

Conclusion: Our findings suggest that extracellular environment is regulated by the UPRmt and any perturbation to it leads to an activation of the UPRmt.

Small Proteins in Pseudomonas aeruginosa

Joanna Idrovo[1], Sarah Park[2], Carl Soderstrom[2], Mona Wu Orr[1, 2]

[1]Department of Biochemistry and Biophysics, Amherst College, Amherst, MA, USA
[2]Department of Biology, Amherst College, Amherst, MA, USA

Introduction: Recent studies indicate that many small open reading frames (sORFs) remain unannotated and were often previously overlooked by bioinformatic and biochemical analysis methods. However, small proteins, defined as less than ~50 amino acids in length, are emerging as important players in many biological processes. Many small proteins are found to be upregulated in changing environmental conditions and often act to modulate the activity, localization, or stability of larger protein complexes. As a highly adaptable environmental bacterial species that is capable of surviving in diverse environmental and infectious niches and as a highly medically relevant opportunistic human pathogen, Pseudomonas aeruginosa it is a prime candidate for novel small protein discovery.

Methods: Using an initiation complex stalling methodology, we have generated a ribosome profiling data set to identify novel sORFs in P. aeruginosa.

Results: Our data show clear ribosome density indicating previously annotated sORFs and we have experimentally confirmed expression of three small proteins via genomic epitope tagging and immunoblotting. One of these is highly conserved in P. aeruginosa strains and co-purifies with a methyl-accepting chemotaxis receptor, although its exact function and mechanism of action remains under investigation.

Conclusion: The aim of this project is to discover novel small proteins encoded in the P. aerugionsa genome, elucidate the function of these novel small proteins, and provide a workflow for the characterization of additional sORFs identified by ribosome profiling.

Development of novel thyroid hormone analog ZTA-261 for hyperlipidemia and obesity

Emily Kim[1]

[1]Nagoya University, Japan

Introduction: In recent years, lipid metabolism related disorders such as obesity, nonalcoholic fatty liver disease (NAFLD), type II diabetes, hyperlipidemia, and cancer have been steadily increasing, leading to a global need for new drugs that help regulate metabolic function. In response, our lab is working to develop and nominate a novel thyroid hormone analog, ZTA-261, for its ability to increase lipid metabolism without concurrent cardiac or hepatic toxicity, a common side effect with endogenous thyroid hormones or previously developed thyroid hormone analogs.

Methods: Our objective this summer was to conduct final experiments in accordance with reviewer suggestions to finalize this paper for publication. As such, we ran three experiments: 1) quantified expression of TH-related genes in addition to general lipid metabolism genes, 2) blood brain barrier permeability assays to assess potential drug side effects, and 3) Mouse femur microCT analysis to determine possible bone deterioration.

Results: We observed a significant increase in gene expression of thyroid hormone related genes when treated with ZTA-261 and low ZTA-261 permeability across the blood brain membrane, and are awaiting microCT scanning and analysis of mouse femur samples.

Conclusion: ZTA-261 was observed to increase gene expression in thyroid hormone related genes to a similar degree as T3 and GC-1, implying that the mechanism by which ZTA-261 and endogenous thyroid hormones function is preserved. Thus, the role of thyroid hormones in the general lipid metabolism process is confirmed, which nominates ZTA-261 as both a novel therapeutic as well as a potential way to further investigate the exact mechanism of lipid metabolism. Secondly, contrary to our expectations, ZTA-261 had a lower permeability than GC-1, though nonsignificant, that was comparable to the negative control. While this eliminates ZTA-261's potential for increasing myelination and oligodendrocyte proliferation in the brain, it also eliminates any cause for concern for adverse side effects, further nominating ZTA-261 a highly favorable pharmaceutical. Lastly, we were unable to finalize microCT analysis of ZTA-261, GC-1, T3, and control treated mouse femurs, but image capture and analysis are an ongoing project in the lab and should yield results within the next 6 months.

High Metal Growth Assays in fpn3 Mutants

Adetola Makun[1], Jeeyon Jeong[1]

[1]Department of Biology, Amherst College, Amherst, MA, USA

Introduction: Iron is an essential micronutrient for nearly all organisms, playing a role in a variety of metabolic processes. Excess Iron can create reactive oxygen species, which can cause damage to cells. Strategy 1 is the reduction-based mechanism for iron uptake under iron deficient conditions.
IRT1, the iron uptake transporter of Strategy I, transports iron but can non-specifically transport other metals into the cell. IRT1 goes through endocytosis and is degraded in high metal environments to avoid toxicity. Ferroportin 3 (FPN3) is an iron exporter in both the mitochondria and the chloroplast fpn3-1 and fpn3-2 are knocked down mutants of FPN3. This poster investigates if fpn3 mutants are more sensitive to high levels of essential non-iron metals.

Methods: This research quantified root lengths of seedlings grown on media containing high non-iron metals. The data includes media with ten times the physiological levels of Zn, Mn, and Co, with the adequate amount of iron for plants, and non-iron media. 15-18 seedlings are used per line to make up each data set.

Results: The data indicates that there is a difference between fpn3- 1 and fpn3-2 under adequate iron conditions. Further studies are necessary to better understand the effect of high non-iron metal under non-iron conditions. Furthermore, the wildtype controls (+Fe and –Fe) are consistent with prior studies, which shows that the procedure worked.

Conclusion: Next steps are to observe phenotypic differences between the same lines under varying levels of added non-iron metals.

Soil Drivers of Arctic Treeline Movement in the Alaska Brooks Range

Ona Ortiz-Gudeman[1], Nife Joshua[1], Rebecca Hewitt[1]

[1]Department of Environmental Studies, Amherst College, Amherst, MA, USA

Introduction: The arctic treeline is the border between the boreal forest and the tundra. The treeline is expected to continue to advance into the arctic tundra, amplifying arctic warming, and further changing the climate (1). The cause of this shift remains unknown, as warmer temperatures alone are not a sufficient cause (1). In the Brooks Mountain Range in Alaska, the treeline is advancing in the Western region, but not in the Eastern (2). This study aims to understand the potential drivers of treeline movement by analyzing the difference in treeline soils from the East and West region of the Brooks Range.

Methods: Soil cores were collected from 3 arctic treelines and 3 alpine treelines at each of 4 Western and 4 Eastern sites in the Brooks Range. In lab, we split each soil core by horizon, into mineral and organic soil sub samples. We then measured and calculated the proportion of rock to soil volume, bulk density, pH, and % moisture content for each soil sub sample.

Results: The results showed significantly lower pH in the Western sites ($p<0.05$), marginally higher rock to soil proportions in the Western sites ($p<0.1$) and no correlation between longitudinal region and bulk density or % moisture content. Arctic treelines had a significantly higher % moisture content than alpine treelines ($p<0.001$), and organic soil had a significantly higher % moisture content than mineral soil ($p<0.001$). Organic soil also had a significantly lower bulk density than mineral soil ($p<0.001$).

Conclusion: These findings are not sufficient evidence to outline the specific abiotic soil factor as a cause of treeline advancement. Next steps could include geologic map data to see if limestone content is the cause of the East vs. West pH difference. More information could be gained from shifting the focus of study to biotic soil variables such as root biomass, mycorrhizal colonization, and fungal species analysis, as well as carbon, nitrogen and phosphorus content.

Iron Homeostasis Gene Expression in Day 7 fpn3-1 and fpn3-2 Mutant Seedlings

Anushka Patel[1], Sara Omer[1], Jeeyon Jeong[1]

[1]Department of Biology, Amherst College, Amherst, MA, USA

Introduction: This research investigates the expression of iron homeostasis genes in Arabidopsis thaliana. Iron is involved in critical processes such as cellular respiration and photosynthesis in plants, and plants must strike a balance to ensure that excessive iron doesn't damage cells. One of the proteins involved with iron homeostasis is FPN3, which is an iron exporter in the mitochondria and chloroplast. Recent work in the lab has analyzed fpn3-1 and fpn3-2 mutations, which are knock-down mutations of the FPN3 gene. The standard in Arabidopsis research has been to study day 14 seedlings, however it has been suggested that gene expression differs in younger plants. This research seeks to determine the expression of various iron homeostasis genes in day 7 fpn3 mutants and determine if there are differences between younger and older seedlings.

Methods: Columbia-0 (Col0, control), fpn3-1, and fpn3-2 seeds are plated on Gamborg's B5 -sucrose agar plates and grown vertically for 4 days. Seedlings were transferred to +Fe and -Fe media on day 4 of growth. Seedling shoots and roots were separated and snap frozen on day 7. RT-qPCR was performed subsequently, and FPN3 shoot and root, MIT2 shoot and root, and IRT1 root expression levels were calculated. Expression levels were normalized to ACT2 (actin).

Results: Preliminary results are consistent with the expected result that FPN3 expression is higher in Col0 seedlings compared to fpn3 mutant seedlings.

Conclusion: More biological replicates (parallel measurements of biologically distinct samples) are required to come to conclusions about the observed results. Future experiments may also include more iron homeostasis genes.

Taste bud expansion in blind Mexican cavefish, Astyanax mexicanus

Isabel Perozek[1], Kaitlyn Reimer[2], Joshua B. Gross[2]

[1]Department of Biology, Amherst College, Amherst, MA, USA
[2]Department of Biological Sciences, University of Cincinnati, Cincinnati, OH, USA

Introduction: The caves of the Sierra de El Abra region of northeastern Mexico are in many ways heterogeneous. The exact nutritional composition and physical environments vary from cave to cave. A few things remain consistent throughout the caves, however, including the lack of light, the lack of food sources, and the lack of predators. These environmental pressures have forced a number of morphological changes in the cave dwelling Astyanax mexicanus, which evolved from surface dwelling ancestors after their invasion of the caves. It is believed that several distinct cave invasions led to multiple instances of the same cave morphotypes in separate locations, including regression of eyes and pigment, as well as the augmentation of taste buds along the dorsal and ventral face and anterior body. How and why taste expansion occurred in the cave morphs is currently unknown. It is hypothesized that this evolved as a mechanism to increase sensitivity to the limited food supply, or as a means of navigation through the dark caves.

Methods: We cloned genes expected to be taste receptor genes and used sequencing data to confirm or eliminate the role of said gene. We performed antibody stains on sections of all four cave populations as well as the surface fish in order to confirm presence and type of extra oral taste bud. Using results from a Quantitative Trait Loci analysis previously conducted in the lab, we determined a genomic interval on chromosome 13 and two genomic intervals on chromosome 2 that are of interest, with three specific genes of interest for future study.

Results: The aim of this project is to characterize the cave fishes' extraoral taste buds and has shown preliminary positive results for T1R1 and T1R3 receptors, suggesting the purpose of perceiving umami flavor in at least one cave population. In our histological studies, we found a difference in the total number of extraoral taste buds between surface and cave fish, as well as a difference in the size of taste buds between different cave populations. We are also interested in determining the genetic component responsible for the expansion of taste buds in the cave populations, and have determined three separate regions of interest spanning two different chromosomes in Astyanax, ripe with candidate genes for further exploration. I have singled out erbb3b, si:dkey151g10.3, and ptprr as specific genes that appear to be associated with functions related to taste or the process of the expansion of the sense.

Conclusion: Determining the structure and location of these genes, as well as the function of taste buds will give us insight into how and why taste expanded in the cave populations, and will offer clues about the nutritional content of caves.

Lung epithelial cells dynamically participate in the immune response to allergens

Phillip Zhou[1], Nicole Case[2], Hadas Pahima[2], Daniel Dwyer[2, 3]

[1]Department of Biology, Amherst College, Amherst, MA, UsA
[2]Brigham and Women's Hospital, Boston, MA, USA
[3]Harvard Medical School, Boston, MA, USA

Introduction: Respiratory illnesses like asthma have historically been thought of as central airway diseases, while the response of the distal lung to such conditions has been less studied. The epithelial cells of the distal airway have also been shown to play a role in the immune response to viral infection, and especially alveolar epithelial type II cells (AT2s). Here, we characterize the response of AT2s when exposed to allergens, identify upregulated transcriptional modules in AT2 cells during allergic challenge, and describe how these modules allow AT2 cells to receive signals as well as influence their surrounding environment.

Methods: To better understand how AT2s sense and influence their surroundings, we used a mouse model of allergy where B6 mice were sensitized to the allergen DerP with the adjuvant Alum, given three intranasal challenges with saline or DerP-containing solution, and sacrificed 72 hours after the last challenge.The lungs were processed for single-cell RNA sequencing, and further in silico analysis was performed in RStudio. To measure surface expression of receptors, we used a pre-existing gating strategy for AT2 cells for flow cytometry.

Results: Our single cell analysis of the mouse lung revealed AT2 cells to be the cell type that responds most dramatically to inflammation as quantified by flow cytometry. Furthermore, AT2 cells can be subdivided into the clusters AT2_D (which expand during allergic inflammation) and AT2_S (cells present at homeostasis). Our differential expression analysis suggests that during allergic inflammation, AT2_D cells gain the ability to sense a wider range of signals, can better present antigens to lymphocytes, and modulate the response of the lung to external signals by production of different intracellular effectors. In particular, it seems AT2 cells become responsive to type 2 cytokine signaling during allergy as suggested by our transcriptomics data, and gain the capacity to produce the anti-inflammatory prostaglandin PGE2 or the pro-inflammatory cytokine IL-33.

Conclusion: This study provides a starting place for investigating AT2 cells as "master regulators" of the distal lung immune response during allergic inflammation and suggests further directions of study for understanding how these cells interact with other components of the immune system like granulocytes and lymphocytes. Our work this summer indicates that further transcriptomics analysis of AT2 cells with bulk-RNA sequencing is required, as well as investigating the interactions of AT2 cells with other cell types in vitro with co-culture experiments.

Chemistry

Synthesizing 2,3-Dicyano-P-Benzoquinone Charge-Transfer Acceptor Molecules

Nina Aagaard[1], Phoebe Eccles[1], Professor Ren Wiscons[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Ferroelectricity is a material property with applications in data storage. The DMDBS-DDQ cocrystal is a charge transfer cocrystal synthesized from a 1:1 ratio of 4,6-dimethyldibenzoselenophene (DMDBS) and 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ). The DMDBS forms a framework of the cocrystal that allows the DDQ to rotate and change states when an external electrical field is applied. The amount of energy necessary to cause this phase change is known as the inversion barrier.

Methods: In this project, we worked on the synthesis of three DDQ analogs, which share a similar structure to DDQ with another element in place of chlorine.

Results: Preliminary testing and further work need to be done before final results are published.

Conclusion: By replacing small amounts of DDQ with analogous molecules (“doping”), we hope to tune the inversion barrier of the cocrystal in order to optimize its data storage capabilities.

The Synthesis of Photoswitchable Naphthalenediimide Derivatives

Brett Donshik[1], Tyler Fields[1], Isabelle Gomez[1], and David E. Hansen[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: The goal of the research pursued was to synthesize the two naphthalenediimide (NDI) derivatives, each of which contains photoswitchable azobenzene amino acid side chains. In nonpolar solvents both derivatives I and II are expected to form supramolecular nanotubes [Pantoş, G.D., Pengo, P. & Sanders, J.K.M, "Hydrogen-Bonded Helical Organic Nanotubes." Angew.Chem. Int. Ed. 2007, 46, 194–197]. These nanotubes may disassemble upon UV irradiation, which will induce the isomerization of the azobenzene functionality from the trans- to the cis-configuration (this isomerization can be reversed by irradiation with visible light or by heating). This photoswitchable disassembly may provide a route to selective release of molecules contained within the pore of the nanotube.

Methods: Standard techniques in organic chemistry were employed in an attempt to synthesize NDI derivatives I and II.

Results: An impure sample of derivative I was obtained, and future work will focus on optimizing the synthesis to obtain pure material. The synthesis of derivative II was unsuccessful, though again work to obtain this molecule will be continued in the future.

Conclusion: We have taken a number of steps towards achieving our experimental aims, but the final results remain to be seen!

Synthesis and Characterization of Zinc Oxide Quantum Dot-Perylene Conjugates

Shani Getz[1], Autumn Y Lee[1], Jacob H Olshansky[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Nanoparticles like quantum dots (QDs) can be used to form donor-acceptor pairs with another molecule, resulting in a well-defined quantum state with two correlated, spatially distant, unpaired electron spins. These correlated spins are called spin correlated radical pairs (SCRPs) and are key to making qubits, the building blocks of quantum computers. This research project studies zinc oxide (ZnO) QDs and their interactions with various perylene dyes as donor-acceptor pairs.

Methods: To better characterize the donor-acceptor system, we focused on (i) evaluating the size dependence of the ZnO on the spin dynamics of the SCRPs and (ii) quantifying the different energies of the perylene dyes and their effect on the system's charge dynamics. We conducted these experiments based on past ZnO QD synthesis notes and literature on electrochemical techniques.

Results: (i) We synthesized different sized ZnO QDs and observed their growth patterns: we discovered that the final ZnO QD diameter was directly proportional to time left stirring and that the ZnO-perylene conjugates should be dried and stored in -22°C to prevent unwanted growth. More data on the spin dynamics of the system will be collected and analyzed in the fall. (ii) We found that the energies of the perylenes were within 0.02V of the predicted values from literature.

Conclusion: This project provides a broader, more quantitative, and more cohesive characterization of the ZnO - perylene donor-acceptor pair system. This work sets a basis for future work with these size-dependent and dye-dependent SCRPs.

Structural Determination of 1,1,2,3,3-Pentafluoroprone and its Argon Complex Using Microwave Rotational Spectroscopy

Maximillian D. Hauschildt[1], Juliane C. Keiper[1], Helen O. Leung[1], Mark D. Marshall[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: In an extension of the Marshall and Leung lab's prior work with halogenated propenes and ethylenes, this research uses microwave spectroscopy to investigate the lowest energy configurations of 1,1,2,3,3-pentafluoropropene (11233-PFP), its carbon-13 isotopologues, and its argon complex. This research will contribute to further comprehension of the relationship between steric and electrostatic factors in formation of non-covalent complexes.

Methods: Ab initio calculations using Gaussian16 at the MP2 level were used to determine the lowest energy structure of 11233-PFP, carbon-13 isotopologues and argon complex structures. A rotational spectrum of 2/3% 11233-PFP/Ar mixture was taken using a broadband, chirped-pulse Fourier transform microwave (FTMW) spectrometer and spectral assignment in PGOPHER based on predicted values from Gaussian determined the rotational constants for each of the structures. The structure of the molecule was adjusted based on experimental rotational constants in STRFIT, and the non covalent interactions within the monomer and between the 11233-PFP-Ar complex were visualized using Multiwfn and ChimeraX.

Results: Analysis of the 11233-PFP structure showed a plane of symmetry and a highly electropositive region near the hydrogen atom. A visualization of the potential energy of different argon orientations around the 11233-PFP molecule was used to find the lowest potential energy structure. Due to the large area at which the lowest energy structure could be located, the calculated lowest energy structure and the observed lowest energy structure were different. The monomer displays simultaneous electrostatic attraction and steric repulsion between the in-plane hydrogen and fluorine, while the dimer shows additional dispersion forces between the argon atom, CHF_2 group and C=C double-bond.

Conclusion: With this research, we add to a fundamental understanding of how steric and electrostatic factors influence non-covalent interactions. Further extensions of this research include the study of the interactions between 11233-PFP and acetylene and a higher resolution spectral analysis to improve the spectral assignment of the current observed species and to detect carbon isotopologues of the 11233-PFP–Ar complex.

Investigating the Synthesis and Catalytic Properties of Single-Initiator Complexes for Ring Opening Polymerization Supported by Phenoxyimine Ligands

Niall Henderson[1], Diane Koo[1], Christopher B. Durr[1]

[1]Department of Chemistry, Amherst College, Amherst, MA

Introduction: This poster represents the synthesis and catalytic properties of titanium IV single-initiator complexes for the ring opening polymerization (ROP) of cyclic esters. Triple-site titanium alkoxide catalysts and their catalytic properties have previously been studied. By collecting kinetic data, it was found that most of the single-site catalysts studied followed a first order coordination insertion mechanism, with the exception of one highly sterically hindered catalyst following a zeroth order mechanism.

Methods: The catalytic synthesis and ROP occurred in an oxygen-free and water-free glovebox at room temperature. For catalytic synthesis, a Schiff base ligand and a titanium alkoxide were combined, with cyclic diol added later. This addition renders the three-initiator intermediate into a single-site catalyst. NMR samples of the catalysts were taken inside the glovebox with Parafilm wrapped at the top. For polymerization, the catalyst and Ɛ-caprolactone were added to a vial and heated to 140C. Aliquots were taken every 10 minutes to track the progress of the polymerization, which was measured in percent conversion to polymer.

Results: The catalysts were found to follow the first-order coordination insertion mechanism, with the exception of one sterically hindered catalyst. The ethoxide catalysts were found to be generally faster than the isopropoxide catalysts.

Conclusion: The single-site titanium alkoxide catalysts behave similarly to their triple-site counterparts.

Optimizing the superfluorescent properties of room-temperature nanoparticles

Kyle Hur[1], Joshua Fung-A-Fat[2], Gang Han[2]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA
[2]UMass Chan Medical School, Worcester, MA, USA

Introduction: Superfluorescence is a unique optical phenomenon that arises from the collective light emissions of excited molecules to produce a short, intense burst of light. The potential applications of superfluorescence include quantum optics and biomedical imaging, thus developing materials that exhibit superfluorescence at room temperature is a prime field of interest in nanotechnology research. This study synthesized KNd2F7 nanowires, tightly packing Nd3+ ions in a crystal lattice to theoretically allow radiative coupling and thus superfluorescence. This study reports the optimal precursor solution quantities and reaction conditions to synthesize KNd2F7 nanowires with promising shape distributions. These findings offer new materials that exhibit superfluorescence, allowing future studies to further investigate the practical applications of superfluorescence at room temperature.

Methods: In a traditional synthesis of KNd2F7 nanowires, Nd(NO3)3 and NH4F is dissolved in deionized (DI) water. Once these compounds are fully mixed, sodium citrate is added, and the reaction mixture is stirred for 30 minutes. Afterwards, KOH is added, and the mixture is stirred for an additional 15 minutes. Then, this solution is hydrothermally treated for 8 hours.
After being cooled to room temperature, the precipitate is collected, washed with 10 mL of DI water, and resuspended.

Results: Dynamic light scattering (DLS) graphs were taken of each sample to obtain the approximate size distributions of the KNd2F7 nanowires. Transmission electron microscopy (TEM) images were also taken to better characterize the shapes and sizes of the nanowires.

Conclusion: TEM showed that samples 6 and 7 were the most promising wire-like nanoparticles. Excess sodium citrate yielded the best nanoparticle shapes. On the other hand, adjusting the reaction temperature affected DLS size distributions, but did not produce more wire-like nanoparticles. These findings establish a protocol for synthesizing new inorganic nanowires and create a pathway to explore superfluorescence for practical applications that have been limited by extreme conditions. Future studies should characterize the superfluorescent properties of samples 6 and 7 with a fluorescence microscope. To synthesize longer nanowires, future trials. should try greater volumes of sodium citrate and reaction temperatures above 200oC. In doing so, superfluorescent materials will hopefully be more accessible and applicable to new disciplines, such as biomedicine and quantum computing, in the foreseeable future.

Synthesis and Characterizations of Single-Site Group V Metal Alkoxides for Catalytic Ring-Opening Polymerizations

Alyssa Huynh[1], Frank Peprah[1], Christopher B. Durr[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Plastics are ubiquitous in modern life, encompassing manufacturing, agriculture, and even medicine.1,2,4 The improper disposal of these plastics, on the other hand, has exacerbated the plastic waste epidemic, putting our ecosystem at risk.1-5 Scientists have made great progress in sustainable plastic waste management over the years, and among those measures, biodegradable plastics represent a promising answer to protect our ecology.5 Ring-opening polymerization (ROP) with metal-alkoxide catalysts can be used to effectively produce biodegradable polymers. So far, aluminum isopropoxide Al(OiPr)3 and group IV metal alkoxides like titanium isopropoxide Ti(OiPr)4 have been widely researched and proved to have the best ROP activity.6 Although less studied, studies on group V metal alkoxide catalysts have also been published.7 The difficulty with these described group V catalysts is that they have many initiator sites, allowing for less-controlled polymerization and reduced molecular weights of polymers.

Methods: 1H NMR, 13C NMR, and single-crystal x-ray diffraction were used to comprehensively describe the complexes. ε-caprolactone (eCL) kinetics were also investigated and reported. 1H NMR and GPC are used to determine conversion rates and molecular weights.

Results: The single initiator site enables controlled polymerization and greater polymer molecular weights.

Conclusion: This work reports the synthesis and characterization of group V single initiator enaminoketonato complexes for ROP.

Controlling Dopant Locale within Mn2+-doped CdSe/CdS Core/Shell Nanoplatelets

Amisha Jain[1], Stephen L. Gibbs[1], Daniel R. Gamelin[1]

[1]Department of Chemistry, University of Washington, Seattle, WA, USA

Introduction: Introducing magnetic dopants within nanostructures results in exchange interactions between the exciton generated from nanostructures and the magnetic ion. These interactions allow for optical control of the ion spin, important for physical implementation of a quantum system. This optical control is greatly enhanced the more central the dopant is within the host lattice; such centrality is achieved via shelling the core nanostructure. Here we incorporate Mn2+ into CdSe core nanoplatelets (NPLs) and investigate the magneto-optical properties given successive CdS shelling.

Methods: Mn2+ locality can be controlled in NPLs via layer-by-layer growth. The previously synthesized CdSe core is 3 monolayers (MLs) thick, after which a Mn2+-doped CdS or CdSe layer is grown around it. Undoped CdS shells are grown one by one around the now 5 ML thick CdSe/CdMnS and CdSe/CdMnSe NPLs. NPLs are characterized after each shelling via absorption/PL and low temperature CW-EPR.

Results: Red shift of absorption spectra upon additional shelling indicates the exciton wavefunction penetrates both the doped CdMnS and CdMnSe layers and leaks into CdS layers. The larger EPR hyperfine coupling constants in 5 ML can be attributed to surface Mn2+ due to electronic interactions with the oxygen of the oleic acid ligand. The decrease in hyperfine constant upon CdS shelling is attributed to internal localization of Mn2+, since it agrees with bulk values.

Conclusion: Exciton wavefunction leakage and Mn2+ internalization are promising trends for increased exciton–dopant wavefunction overlap and thus increased exchange interactions. Future work involves quantifying exciton–dopant interactions via magnetic circular dichroism (MCD) in CdSe/CdMnS and CdSe/CdMnSe NPLs. Additionally, we wish to investigate replacing CdS MLs with CdSe to perhaps maximize wavefunction overlap.

Quantifying Hydroxyl Radicals Generated by Photoexcitation of a Synthetic Melanin Using Terephthalic Acid as a Fluorescent Dosimeter

Zoe Jonas[1], Bárbara Fornaciari[1], and Bern Kohler[1]

[1]Ohio State University, National Science Foundation

Introduction: Melanin is a ubiquitous pigment found throughout nature that is responsible for the color of skin, eyes, and hair in humans. Melanin occurs naturally as nanoparticles, but the underlying molecular-level structures are uncertain. While eumelanin is best known for its sun-screening properties, continuous exposure to ultraviolet or visible radiation results in the production of reactive oxygen species (ROS), which are deleterious oxygen-containing molecules that can impair cellular functions through oxidative stress.

Methods: Terephthalic Acid, TA, is one of many probes used to detect these ROS. TA does not fluoresce on its own but it does emit in the blue wavelengths when in the presence of ·OH hydroxyl radicals. This fluorescence allows the production of ·OH to be quantified. The increase in blue emission at 440 - 490 nm is due to the production of hTA, which is a TA molecule with the addition of an OH, during irradiation. This curve allowed the quantum yield of hTA in aqueous solution to be calculated based on the known QY of 2-aminopurine (2-AP).

Results: The resulting QY is 66%. Because optical density influences the quantification of hTA and, consequently, the amount of HO• radicals formed, the concentration of hTA formed was calculated at OD = 0.41. Considering the efficiency of the reaction of TA + HO• to be 30%, the estimated concentration of radicals photoproduced is approximately 8 mmol of HO• per mol of melanin monomers, after 24 h of irradiation. However, this ratio is specific to the light source used.

Conclusion: Further experiments using chemical actinometry must be performed to estimate the quantum yield of HO• radicals.

Trinitrotriphenylamine Synthesis and the Significance of Sumanenes

Tristan Kim[1], Alex Da Rosa[1], Carley Daly[1], Professor Ren Wiscons[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: This research poster showcases the potential for Sumenenes as organic ferroelectric molecules with data storage capabilities. The synthesis of Sumanenes begins with the formation of Trinitrotriphenylamine and its subsequent reduction. Both of these protocols were studied, performed, redesigned, and optimized so that one might continue in the next synthetic step.

Methods: Using a broad range of procedures including overnight reactions, extractions, filtrations, and centrifuging, one can successfully synthesize Trinitrotriphenylamine and then reduce its nitrous groups into amine groups. Quantitative data and yield can be collected at each step after recording the respective masses of starting materials. Augmentations to the protocol were implemented as seen fit in an effort to optimize the reaction.

Results: Aside from visual indications such as color changes and formation of precipitate, a successful synthesis of Trinitrotriphenylamine can be determined through a Nuclear Magnetic Resonance of the product dissolved in a solution of Deuterated Chloroform. Similarly, a successful reduction of Trinitrotriphenylamine can be verified by NMR when dissolved in Acetone. The reduced product should also show a double peak at around 3500 cm-1 wavenumber on an Infrared Spectrograph. The NMR of the Trinitrotriphenylamine was unclear, likely due to interference from unwanted extraneous products. The color changes were promising, but it is likely that the protocol needs to be further modified in order to yield cleaner results. However, the IR of the reduced product showed a distinct double peak in the desired area, indicating a somewhat successful reduction.

Conclusion: The work-up protocol of the initial synthesis demands the greatest amount of attention both in terms of time and reaction sensitivity. The 4 hour segment in which the work-up is performed has shown to have the greatest variability in results, and thus required many modifications to the respective portion of the protocol. However, the color changes and the results of the reduction indicated some levels of successful product formation, and with minimal adjustments the initial steps can be optimized and more consistent so that the synthesis can continue towards the ultimate goal of creating Sumanenes.

Exploring Intermolecular Interactions: The 3,3,3-Trifluoropropene···Argon Complex

Luke N. Kline[1], Pohakea G. Mawyer[1], Helen O. Leung[1], Mark D. Marshall[1]

[1]Department of Chemistry, Amherst College, MA, USA

Introduction: How can we better understand the intermolecular forces that drive chemical interactions? How can we measure the structures of molecules down to a hundredth of an angstrom? To answer both of these questions, we turn to the powerful tool of microwave rotational spectroscopy. This research investigates 3,3,3-trifluoropropene (333TFP) and its argon complex. 333TFP is a particularly interesting molecule because of its intense dipole moment and electronegative trifluoro group, leading to strong measurements in a spectrometer and fascinating interactions with argon. Through determining the structure of 333TFP and its argon complex, we hope to expand our understanding of intermolecular forces in olefins.

Methods: This study combines theoretical ab initio calculations with an experimental spectrum to determine the precise structure of 333TFP and its argon complex. To start, the structure of 333TFP along with its moments of inertia and dipole moments are predicted using the Gaussian 16 program. A sample of 333TFP in argon is then put into a microwave spectrometer, and is exposed to frequencies ranging from 2.0 to 18.1 GHz. The calculated moments of inertia are used to predict the frequency required for 333TFP to transition from one rotational energy level to another. By adjusting the calculated moments of inertia to match the experimental data, it is possible to find precise bond lengths for 333TFP down to a hundredth of an Angstrom.

Results: Due to the robust dipole moment, uncharacteristically strong a-type transitions were observed in the monomer. In addition to creating a fascinating spectrum, these strong transitions also proved crucial in locating the 13C isotopologues of the monomer. The Ar dimer has intense b-type transitions, allowing 320 total transitions to be observed in the most abundant species with an additional average of 46 transitions per 13C isotopologue. Excitingly, the 36Ar isotopologue, which had not yet been seen in our lab, was potentially observed in the 333TFP spectrum due to the sheer strength of the b dipole moment.

Conclusion: The structures of 333TFP and its argon dimer give insight into the intermolecular interactions that glue these molecules together. In the monomer, there is an internal hydrogen bond between a fluorine atom and a hydrogen atom that holds the trifluoro group in place and provides a high energy barrier to internal rotation. In the argon dimer, there is a primary interaction between the argon atom and the aforementioned fluorine atom, and a secondary interaction between the argon atom and the π electron density of the C=C double bond. The findings of this study are consistent with similar studies and will serve as an important data point for future research in the field.

Mass Spectrometry Analysis of Myoglobin Unfolding in Acetonitrile

Taylor Malone[1], Jackson Lee[1], Sheila Jaswal[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Apo-myoglogin's folding has been extensively studied and modeled. However, while experiments have also looked at the unfolding of holo-myoglobin, this process is complicated by mixed protein populations due to the dissociation of heme.

Methods: Mass spectrometry can easily differentiate apo versus holo myoglobin but the technique is incompatible with traditional chemical denaturants like urea and guanidine. However, acetonitrile can be used to denature proteins and it is compatible with mass spectrometry. Experiments were conducted to measure changes in mass spectrometry charge state distributions as a function of acetonitrile concentrations for holo-myoglobin.

Results: Data revealed the changes in the populations of apo and holo myoglobin as the protein unfolds. Holo-apo dimers and higher order oligomers were also detected as the protein unfolds.

Conclusion: Acetonitrile denatures myoglobin similarly to traditional denaturants. This indicates its prospective utility as a denaturant for use in studying the kinetic and thermodynamic parameters of protein folding and unfolding, especially combined with its potential for use in HXMS experiments.

Polypeptides as Biodegradable 3D Printable Materials

Holden Orias[1, 3], Ronnie V. Garcia[2, 3, 4], Craig Hawker[2, 3, 4, 5]

[1]Amherst College
[2]Department of Chemistry & Biochemistry, UCSB
[3]Materials Research Lab, UCSB
[4]BioPacific MIP
[5]Materials Department, UCSB

Introduction: Modern biomedicine calls for easily-producible solutions to patients' individual needs; additive manufacturing addresses this need through a blend of scale and customization. Current widely-used bioinks, however, either lack synthetic tunability or are not biodegradable (gelatin and poly(ethylene glycol), respectively). Therefore, advancing the technology requires a broader selection of biologically compatible and tunable materials. Polypeptide hydrogels hold particular interest for their biodegradability in physiological conditions, especially because of their tunable rate of degradation.

Methods: A novel gel network was synthesized from a dye-conjugated polypeptide. The network was then subjected to both chemical and biological degradation conditions, with the degradation pathway characterized through fluorescence spectroscopy.

Results: Under chemical conditions, the polypeptide network degraded more rapidly than it did in biological conditions. Both conditions, however, showcased the network's significantly higher structural integrity compared to that of the gelatin network, supporting the use of polypeptide hydrogels as a high-fidelity degradable bioink.

Conclusion: Further characterization of our system's degradation kinetics will constitute additional progress toward the development of bioresorbable implants and advanced drug delivery systems.

Synthesis of Photoluminescent ZnTe/ZnSe Quantum Dots for Photocatalytic CO2 Reduction

Caleb J. Savoie[1] , Frida Hernandez[1], Jacob H Olshansky[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: This project tested various methods of synthesizing photoluminescent ZnTe/ZnSe and ZnTe/ZnSe/ZnS Quantum dots. Higher temperatures and adding a ZnS shell produce a more stable Quantum dot structure. We hope that these dots will provide a viable cadmium-free option for CO2 Reduction.

Methods: This study combined procedures from previous ZnTe/ZnSe Quantum dot syntheses with new strategies. The goal was to create a synthesis that produces photoluminescent, water/air-safe, cadmium-free quantum dots. Ultraviolet-Visible spectroscopy and a fluorimeter provided quantitative data on the shell growth.

Results: This experiment showed that ZnTe/ZnSe and ZnTe/ZnSe/ZnS Quantum dots synthesize best in a nitrogen atmosphere at 230℃. Slow injection of Zinc Oleate and Selenium-Trioctylphosphine simultaneously over two hours grew more stable shells than the Successive Ionic Layer Adsorption and Reaction (SILAR) method. Using Ultraviolet-Visible spectroscopy, the ZnTe Quantum dot cores had a peak absorbance of around 430 nm, while the final ZnTe/ZnSe/ZnS QDs had a peak absorbance of 508 nm. The redshift provides evidence of shell growth. Transmission electron microscopy confirmed this growth. The ZnTe QD cores had a diameter of 2.8 ± 0.7 nm, the ZnTe/ZnSe QD's had a diameter of 3.7 ± 0.7 nm, while the ZnTe/ZnSe/ZnS QD's had a diameter of 4.9 ± 0.7 nm.

Conclusion: In conclusion, this study provides a procedure that produces photoluminescent ZnTe/ZnSe/ZnS Quantum dots. We discovered photoluminescence depends on temperature during synthesis. At around 200℃, the QDs did not fluoresce under UV light, while at 230℃, they did. With continued research, a zinc-based quantum dot can provide a less toxic alternative to cadmium-based quantum dot CO2 Reduction.

Structure Determination of 3-fluoropropene and its Argon Complexes via Microwave Rotational Spectroscopy

Colin J. Sueyoshi[1] Ashley C. Yuen[1], Helen O. Leung[1], Mark D. Marshall[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Microwave rotational spectroscopy is an analytic technique used to determine the structures of molecules and their complexes. Continuing our lab's work on halogenated propenes, we seek to determine the structure of 3-fluoropropene (3FP) and explore its interactions with argon.

Methods: Ab initio calculations were performed using Gaussian 16 software at the MP2 level of theory to predict structures and rotational constants, giving a rough approximation for peak locations. A 2.0-18.1 GHz spectrum of 2/3% 3FP in Ar was obtained using a chirped-pulse Fourier transform microwave spectrometer. Peak assignments were completed using Western's PGOPHER software to obtain experimental rotational constants. Bond lengths, angles, and dihedral angles were calculated from experimental constants using Kisiel's STRFIT, and the Cartesian coordinates of the fitted structure were compared using Kisiel's KRA program.

Results: Potential energy scans of the –CH2F rotamer yielded two unique rotamers: gauche and cis. Peaks for both rotamers were identified and assigned on the experimental spectrum. 6 parameters were fitted to the 12 rotational constants of the parent and all 13C isotopologues for each rotamer to obtain experimental structures for the monomer. Scans of argon around the center of mass of each rotamer resulted in 2 minima for the gauche rotamer and 1 minimum for the cis rotamer. However, only one structure for each rotamer was observed on the experimental spectrum. After obtaining rotational constants from argon complex isotopologues, argon positions were fitted, giving final structures of the Ar-3FP complex.

Conclusion: Theory was a good prediction for our 3FP monomers and complexes, as the difference between the predicted and experimental structures and rotational constants were small. We observed two rotamers – cis and gauche – and obtained experimental structures for their monomers and argon complexes.

A Spectroscopic Study on Forces: Argon – 3-chloro-3,3-difluoropropene

Kazuki M. Tayama[1], Helen O. Leung[1], Mark D. Marshall[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Spectroscopy is a tool utilizing electromagnetic radiation (light) to study various properties of molecules. In the microwave (MW) range, rotation properties determine interactions with light. Since the mass and its distribution determine how anything rotates, we can use such information to study structure. Following the implementation of supersonic expansion to MW spectroscopy in the mid-late 20th century, it has become the preferred tool to study intermolecular forces through weakly-bound dimers between two molecules. Halopropenes are simple, small molecules with very electronegative atoms, making them ideal to continue such studies, and include 3-chloro-3,3-difluoropropene (3Cl33DFP), best considered in direct comparison to other molecules of ongoing study such as 3-fluoropropene and 3,3,3-trifluoropropene.

Methods: A chirped-pulse Fourier transform microwave spectrometer is used to obtain the 2.0-18.1 GHz spectrum of ⅔% 3Cl33DFP in argon (Ar) carrier gas. The spectral analysis was first guided by computational chemistry: calculations using an ab initio method (MP2) were conducted using Gaussian 16. Visualizing both the observed spectrum and calculated spectrum using Western's PGOPHER, calculated transitions were assigned to observed peaks and then processed using Pickett's SPFIT. Using the parameters obtained from this analysis, structure determination was conducted with Kisiel's STRFIT.

Results: The presence of different atoms on the rotatable -CClF2 group suggests the possibility of two stable configurations relative to the C=C double bond, named gauche and cis by where the Cl lies. Computations suggest the cis rotamer is less stable, reciprocated by much weaker peaks in the spectrum. Observed are peaks corresponding to the Cl-35 and Cl-37 isotopologues of both rotamers of the 3Cl33DFP monomer, as well as the Ar – 3Cl33DFP-gauche dimer. Additionally, all single C-13 isotopologues of the gauche monomer were found and analyzed. Unfortunately, the Ar – cis complex was not observed, so a direct comparison of experimental bond lengths with the gauche analogue was impossible. Regardless, in accordance with theory predicting the general Ar binding mode correctly in most cases, we still use the theoretical structures to understand the intermolecular forces better.

Conclusion: MW spectroscopy was used to study 3Cl33DFP's rotamers and their Ar dimers. The study most importantly serves as a base to start studying interactions of 3Cl33DFP with protic acids like acetylene. However, the Ar dimer remains interesting, as we observe that Ar chooses to bind to Cl rather than the more electronegative F in the gauche dimer, reflecting Cl's higher polarizability and its electrostatic potential that allows a stronger Ar interaction with the C=C bond.

New sorbent platforms for humidity-swing direct air capture

Maggie Yang[1, 3, 4], Benjamin Shindel[2, 3, 4], Noryana Nano[2, 3, 4], Vinayak P. Dravid[2, 3, 4]

[1]Amherst College
[2]Northwestern University Department of Materials Science and Engineering
[3]Northwestern University Atomic and Nanoscale Characterization Experimental Center (NUANCE)
[4]Northwestern University Soft and Hybrid Nanotechnology Experimental Resource (SHyNE)

Introduction: Global warming dramatically impacts our ecosystems and communities, impacting water and food resources, human health, and the environment. This work investigates various materials that can be used for carbon capture via moisture-swing processes. By using humidity changes to facilitate carbon dioxide (CO2) capture and release, the process avoids the need for drastic temperature changes and significant amounts of energy. We aim to find new materials that are more efficient, cost-effective, and synergistic with other types of CO2 capture and conversion.

Methods: Here, we test various novel moisture-driven CO2 sorbents, which selectively capture CO2 under dry conditions and release it under wet conditions.

Results: The tuning of humidity promotes the at-will adsorption and desorption of CO2, allowing for the repeated use of the sorbent material over multiple cycles. We use microscopy and spectrometry techniques to characterize our synthesized materials.

Conclusion: This study presents new sorbent platforms that exhibit moisture-swing effects, allowing further investigation and comparison with other materials for the purpose of large-scale carbon capture.

Synthesis and Quantum Yield of Indium Phosphide Based Quantum Dots

Stella Yuan[1] and Kaela Liu[1]

[1]Department of Chemistry, Amherst College, Amherst, MA, USA

Introduction: Quantum dots are metallic nanocrystals that are so small that they act like a single atom and fluoresce different colors depending on their size. They have applications in areas such as bioimaging, LEDs, and photocatalytic energy conversion. However, many mainstream quantum dots contain cadmium, an extremely toxic cancer-causing metal. This summer, we synthesized indium phosphide (InP) based quantum dots as a safer alternative to cadmium metal and tuned their core sizes and shell thicknesses. Furthermore, we analyzed how effectively the InP-based dots emit light by calculating their quantum yield and analyzing their photon emission processes. We considered how altering techniques, chemicals, and shells changed the dots' efficiency. In the long term, we aim to achieve versatile methods to synthesize quantum dots of all different colors and varying shell thicknesses.

Methods: Our synthesis of InP-based dots followed portions of the procedures described in an ACS Nano article by Hannes Van Avermaet et al. titled "Full-Spectrum InP-Based Quantum Dots with Near-Unity Photoluminescence Quantum Efficiency." Following the first synthesis, we experimented with ways to shorten the procedure while still obtaining a good quantum yield. We attempted to grow dots with different intermediate shell thicknesses and grew an additional outer shell on one of our samples. With all of the samples, in order to determine their quantum yield, we measured their absorption using UV-Vis spectroscopy and measured their emission and excitation at a number of different wavelengths using a fluorescence spectrophotometer. In addition, we took time-resolved photoluminescence (TRPL) readings of the dots to collect data on their various photon emission processes. Lastly, we measured the size of all our quantum dot samples using transmission electron microscopy (TEM).

Results: We found that growing one intermediate shell with different ratios of selenium to sulfur was less effective than growing an ZnS outer shell on the intermediate shell. In addition, quantum dots with the same core compositions showed nearly identical core emission wavelengths and core absorptions. Lastly, there was little correlation seen between overall quantum dot size and quantum yield. This is most likely due to the fact that quantum yield is also highly dependent on both shell thickness and core composition.

Conclusion: Our project this summer provided the lab with useful initial methods for synthesizing successful InP-based quantum dots that can be used for future projects. By replacing our cadmium based quantum dots with InP-based quantum dots we are making the lab environment a safer place as well as making the dots more versatile for use in applications such as bioimaging.

A New Visualization Framework for NVMExplorer to Compare the Performance of Memory Technologies

Javier Gutierrez Bach[1], Lillian Pentecost[1]

[1]Department of Computer Science, Amherst College, Amherst, MA, USA

Introduction: With exponential growth in the computer science landscape, data-intensive algorithms such as DNNs (deep neural networks) or graph processing have become too much of a burden on the memory technologies we use. To overcome the efficiency and latency limitations that current memories (SRAM, DRAM) have, embedded non-volatile memory technologies (eNVMs) were proposed. NVMExplorer is an open source design space exploration (DSE) framework which, based on circuit and device parameters, system constraints, and application level behavior, provides statistics on these different memory cell configurations' performance. Despite this, it does not provide guidance or tutorial materials for the user to contextualize their results. The newly presented work, 'NVMExplorer: Story Mode', allows the users to visualize their data in a cross-computing-stack narrative, accompanied by helpful texts and data filtering according to the user's priorities. With both tools, a researcher might be able to answer many research questions on which memories are better for certain applications.

Methods: The new platform is built off of the python libraries of pandas, numpy, matplotlib, and the ipywidgets resources from Jupyter Notebook. This visualization guide will be made available open-source with options for users to add their own data. Moreover, the user will have toggles for all of the memory cell types and other configuration parameters, so that the user can choose when to see results corresponding to each cell dynamically. Similarly, there are sliders to personalize the ranges of values shown in the graphs, both in a linear and exponential manner, to allow for a more focused analysis.

Functionality: The main accomplishment of this project is the guided narration of the data. It starts off illustrating device-level statistics so that the user understands how each cell configuration acts amidst different conditions. This becomes necessary to understand information presented in later chapters of the guided tool. The second chapter looks at how the memory array works in an ordinary computer's workload. That is, how the latency, energy per second might vary per memory type for different traffic patterns. Lastly, the user will classify these patterns into application buckets like DNNs or graph processing, and compare the performance of each cell for the different data-intensive applications.

Conclusion: In essence, this research commends the use of 'NVMExplorer: Story Mode' to fully comprehend and create conclusions about your NVMExplorer data. As commented, the features and implementation facilitate a learning experience for personalized research questions and can help software developers optimize the performance of their projects, posing a benefit to the computer science community.

Understanding Neural Networks Using DFAs

Margaret Bailey[1], Professor Alfeld[1]

[1]Department of Computer Science, Amherst College, Amherst, MA, USA

Introduction: A Deterministic Finite Automaton (DFA) is a machine that accepts a set of strings. DFAs are very simple computational machines, and therefore are well understood.

Methods: This summer, we studied an algorithm that, given the ability to query an input DFA, produces an equivalent DFA. We hope to modify this algorithm to generate a DFA that models a neural network (a type of predictive machine that classifies data).

Results: In contrast to a DFA, a neural network is trained on data and changes over time, so it is more difficult to understand the internals of a neural network, as it isn't set at the beginning. Since we better understand the internal behavior of DFAs than neural networks, finding one that models a simple neural network may help us gain insights into understanding how neural networks work.

Conclusion: We plan to start with a simple neural network that distinguishes between two classes, and if this is successful, train it on more classes.

Building User-Centered ASL Communication Technologies for Parent-Child Interactions

Ashley Bao*[1], Kaleb Newman*[2], Madeleine Mann[3], Ekram Hossain[4], Chigusa Kurumada[5], Zhen Bai[4]

[1]Amherst College, Amherst, MA, USA
[2]Brown University, Providence, RI, USA
[3]University of Rochester, Rochester, NY, USA
[4]Department of Computer Science, University of Rochester, Rochester, NY, USA
[5]Department of Brain and Cognitive Sciences, University of Rochester, Rochester, NY, USA
*These authors contributed equally.

Introduction: Since most deaf or hard-of-hearing (DHH) children are born into hearing families, they are at risk of lifelong language deficits from a lack of natural language exposure in early childhood. The Tabletop Interactive Play System (TIPS) is a real-time American Sign Language (ASL) communication aid, for face-to-face joint play between hearing parents and their DHH children. We investigate user preferences for different ASL recommendation methods, providing insights into optimizing ASL communication technologies for hearing parent-DHH child interactions.

Methods: We introduce Tap-to-Sign, a novel AR projection-based ASL sign retrieval system that grants parents complete control over the recommended word to sign to their DHH child. Additionally, we propose three distinct automatic recommendation strategies, drawing insights from language acquisition research: part-of-speech, semantic weight, and word prevalence. To gain insights into our diverse methods, preliminary feedback was gathered from key stakeholders through a semi-structured interview.

Results: In preliminary feedback from a language development expert and an undergraduate student, neither of whom had prior experience with ASL, we found that participants generally liked Tap-to-Sign, but expressed concerns about disruptions to the flow of interaction when playing with a child. They had diverse preferences on the three different automatic recommendation strategies, indicating that future work may focus on customizing TIPS to the individual user.

Conclusion: Our team previously presented TIPS, a communication aid that addresses a critical need to improve the quality of communication between DHH children and their hearing families. Now, we introduce Tap-to-Sign and three automatic ASL recommendation strategies: part-of-speech, semantic weight, and word prevalence. These novel systems allow us to tackle the question of what words the system should expose to parents and children. We gathered preliminary feedback on our system which indicated that different users will have different preferences regarding Tap-to-Sign and the different automatic recommendation strategies. Moving forward, we plan to conduct a full feedback study with stakeholders and then conduct a user study with hearing parents and their DHH children.

The Impact of ChatGPT on Consultants

Kevin Dai[1, 2] Fabrizio Dell'Acqua[2], Edward McFowland III[2]

[1]Amherst College, Amherst, MA, USA
[2]Harvard Business School, Boston, MA, USA

Introduction: Generative artificial intelligence (AI) tools, such as those built upon generative pre-trained transformer (GPT) language models like ChatGPT, have rapidly become one of the most influential topics in business. Their potential to displace jobs and revolutionize the way that people work could have large-scale implications for the future of many organizations and subsequently the economy.

Methods: By partnering with a large consulting firm in this project, we conducted a large-scale randomized controlled experiment to evaluate the usefulness of generative AI as a tool for writing and problem-solving tasks, investigating how the use of GPT impacted performance on functions relevant to the daily work of consultants.

Results: For both tasks, our work found that most respondents given access to GPT retained a significant portion of the content that GPT returned to them in its responses, with users often choosing to copy the text in its entirety while only making minor modifications. This led participants assigned the writing task with access to GPT to score substantially higher than their previously measured baseline performance and higher than a control group without access to GPT. However, it also led to worse performance for those given access to GPT in the problem-solving task since GPT would often lead the user to an incorrect solution. In both cases, access to GPT significantly reduced the amount of time that participants spent on the given tasks, suggesting the potential for increased productivity when leveraged properly as a companion for human workers.

Conclusion: The next phase of this project involves another experiment that explores how generative AI might augment the skills of data scientists, where individuals are already technically fluent. These findings help demonstrate the potential influence of generative AI on high-skill professions and better inform business leaders about how companies can leverage AI in the workplace.

Optimization of the WK Compression Algorithm

Sam Fetters[1], Lynca Kaminka[1], Scott F. Kaplan[1]

[1]Department of Computer Science, Amherst College, Amherst, MA

Introduction: This study explores the WK cache compression algorithm, which stores virtual memory pages in compressed form by leveraging data patterns. It maintains a recency based dictionary (of 4-16 words) implemented via direct-mapped or fully associative structures. The goals of this study included assessing potential improvements from 64 or 512 bit packing sizes, as well as the impacts of different dictionary structures and sizes.

Methods: Compression has two phases: modeling, where the algorithm evaluates words against the dictionary, assigning tags indicating the location of the words' bits, and packing, which encodes the tags, the sequence of lower bits, and the sequence of dictionary indices. Decompression sees this sequence reversed, with unpacking first, followed by un-modeling. This research tested the algorithm with four traces of varying sizes from a computer system, and studies the utilization of its components during execution.

Results: The results of this research indicate significant time improvements with a direct-mapped dictionary, as compression/decompression time relative to compression size remains near-constant with the former as opposed to a linear association with a fully-associative one. As for dictionary sizes, smaller sizes consistently resulted in quicker compression and decompression. Finally, while compression/decompression times remain fairly constant regardless of packing word size, packing/unpacking times are in some cases 75-90% faster with 512 bit packing than the alternatives, indicating greater efficiency.

Conclusion: An optimized implementation of the WK algorithm should run with a 512 bit packing size, and a direct-mapped dictionary with a size of 4. However, while 512 bit packing has an impact on packing/unpacking times, it's diminished over the rest of the algorithm, as is dictionary size with a direct-mapped dictionary. Ultimately, the organization of the dictionary plays the largest part in deciding the algorithm's speed. For future work, focus should be placed on speeding up the modeling and unmodeling, as they take up the bulk of compression and decompression time.

Memory of the Future: Simulations of Emerging Embedded Non-Volatile Memories (eNVMs)

Sandesh Ghimire[1], Shinsaku Kataoka[1], Lillian Pentecost[1]

[1]Department of Computer Science, Amherst College, Amherst, MA

Introduction: The exploration of emerging embeddable non-volatile memories (eNVMs) such as FeFET, PCM, RRAM, and STT-MRAM, over the last three years, offers a glimpse into the continuing evolution and innovation of memory technologies. This study dives deep into their potential to supplant conventional memories such as SRAM and DRAM by modeling and evaluating recent advances against standards from prior work based on 2016-2020 publications. Using DNN benchmarks, we also assess how these eNVMs can be optimized to improve the power efficiency of modern computing tasks.

Methods: We reviewed eNVM papers from ISSCC, IEDM, and VLSI (2020-2023) and extracted cell configuration data. Based on the obtained data, we used NVMExplorer to model array-level characteristics. We then simulated eNVMs against six primary criteria focused on energy, density, and power optimization. Our analysis covered key metrics like Read Latency vs. Read Energy, Write Latency vs. Write Energy, and Area vs. Area Efficiency. We validated our simulations against fabricated test chips and assessed their use in DNNs using ResNet26, storing weights and/or activations in a 2MB memory.

Results: Using NVMExplorer, we evaluated key metrics across eNVMs at 1MB based on published cell characteristics from 2020-2023 and compared them with optimistic and pessimistic projections from 2016-2020 publications. Our analysis revealed that recent FeFET examples outperform past pessimistic cell assumptions in area and align with optimistic ones. Advances in PCM showed reduced read latency and energy consumption, surpassing even the optimistic prior estimates, while recent STT-MRAM progress has boosted energy efficiency and write speeds, consistently aligning with optimistic predictions. To assess recent eNVM configurations as potential SRAM replacements in deep learning accelerators, we analyzed 2MB capacity eNVM arrays under ResNet26 traffic patterns, focusing on DNN inference simulations with only weight storage, resulting in read-only traffic during inference, and which meet the software requirement of completing 60 frames per second. Comparing optimal eNVM choices for DNN benchmarks based on simulation results from 2016-2020 and 2020-2023 publications, we observed that FeFET has become the optimal choice for all benchmarks in terms of area. PCM remains dominant for weights-only benchmarks, while RRAM surpasses STT-MRAM as the preferred choice for weights-and-activation benchmarks.

Conclusion: Our study advocates for eNVMs as potential successors to conventional memory systems. Simulations reveal FeFET's superiority in terms of area, power efficiency, and DNN application, while PCM, STT-MRAM, and RRAM show improved energy, latency, and reduced DNN inference power respectively.

Language Models as Interpreters: Can LMs Describe the Behavior of Black-box Functions?

Reihaneh Iranmanesh[1], Sarah Schwettmann[2, 3], Jacob Andreas[2]

[1]Department of Computer Science, Amherst College, Amherst, MA, USA
[2]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA, USA
[3]Department of Brain and Cognitive Sciences, Massachusetts Institute of Technology, Cambridge, MA, USA

Introduction: Recent research highlighting the advanced reasoning and problem-solving capabilities of language models (LMs) across multiple domains implies their potential to serve as a general-purpose interface for interpretability. Interpretability in this context is the capacity to elucidate the mechanisms through which these complex neural networks generate outputs and identify influential factors within their input data. However, measuring LMs' performance on interpretability tasks is challenging due to the inherent difficulty of quantifying those tasks and the absence of known ground truth.

Methods: To address these issues, our lab has previously established a first-of-its-kind benchmark for evaluating function interpretations and interpretability methods, catalyzing my research on enhancing LMs’efficacy as interpreters. My efforts were mainly channeled toward using Vicuna, an open-source LM, as a backbone for implementing synthetic neural modules and developing a tree-of-thoughts (ToT) problem-solving pipeline for interpretability tasks.

Results: Post-training, Vicuna excels on all out-of-domain (OOD) instances in the test set for both clean and corrupted functions. However, due to deliberate overfitting, Vicuna's accuracy on clean functions declined from 83.8% to 80.5%, reflecting a loss of some general knowledge, specifically in in-domain instances. Moreover, the model falters with complex OOD examples in corrupted functions outside of the test set, suggesting that we need to include more complex and nuanced OOD training examples to improve model robustness and generalization capabilities. We also plan to utilize weight regularization techniques and integrate Vicuna-specific training examples in our training data to preserve general knowledge and prevent overfitting. My findings also suggest that a ToT structure leads to superior hypothesis generation and instruction-based interpretations. Thus, ToT has the potential to avoid confirmation bias by ranking different hypotheses and selecting the best ones.

Conclusion: In time, these efforts will culminate in developing a multimodal (vision and text) large interpretability model (LIM). By possessing greater interpretability competencies in explaining the behavior of various black-box functions, including neural modules, LIM has significant potential to promote transparency in AI decision-making processes. Additionally, our study sets a solid groundwork for future research in mechanistic interpretability.

A Grade Solution: Minimizing Wait Times at Starbucks with QR Codes

Tairan "Ryan" Ji[1], Kristy Gardner[1]

[1]Department of Computer Science, Amherst College, Amherst, MA, USA

Introduction: Humans spend a significant amount of their lives waiting in lines, often in fast-food restaurants. By improving the policy of how lines are managed, we can reduce waiting and have more time for the things we care about. One potential improvement is allowing customers to place orders with QR codes. Our project simulates the impact of implementing QR in Starbucks under three different policies to gain a preliminary understanding of the technology's potential for the entire fast-food industry.

Methods: The computer simulation, with parameters based on prior research and public information from Starbucks, models a generic store that originally only supported mobile, drive-through, and in-store ordering with cashiers but recently introduced QR ordering. The three policies tested ("Baseline," "QR Favoring," and "QR First") differ in how much baristas prioritize QR orders, with Baseline giving no priority and QR First giving as much priority as possible. Since Baseline functions almost as if QR ordering doesn't exist, it is used as a control to measure the effectiveness of the other two policies. Each policy was simulated multiple times at different customer arrival rates.

Results: QR ordering implemented under QR First demonstrates the potential to reduce waiting. The policy created extremely low barista average response times (time from order placement to order completion) for QR at the slight expense of other orders. Although the policy doesn't affect the overall barista average response time (average of the response times of all order types), it significantly incentivizes in-store customers ordering with cashiers to switch to QR. This reduces time spent waiting to order because QR can serve an unlimited number of customers simultaneously while the number of cashiers is limited.

Conclusion: The results prompt two general directions for future research. The first will involve expanding and refining our simulation of Starbucks with efforts such as testing more policies that may be more effective and collecting real-world data to produce more accurate simulation results. The second direction will involve generalizing ideas from our findings to not only the fast-food industry but also beyond: QR eliminates waiting by directing customers to serve themselves (place orders) with their own resources (their phones), so it may be productive to identify applications for QR and other technologies that share this property in other industries.

Data Pipelines for a Museum: The Wistariahurst Case

Matteo Riondato[1], Ris Paulino[1], Sarah Wu[1]

[1]Department of Computer Science, Amherst College, Amherst, MA, USA

Introduction: This research focused on improving accessibility to museum documents for archivists and the general public. We worked with the Wistariahurst Museum in Holyoke, MA in order to better meet their needs.

Methods: Looking at the thirteen finding aids the museum sent us, we looked at the formatting, word choice, and overall similarities between the documents in order to develop general-use data extractors.

Results: We created a data pipeline and developed software to convert, compress, and standardize information from Wistariahurst's Collection Finding Aids document. We stored the extracted information in JSON, a universal data format that is both human- and machine-readable. From JSON, information would be easily converted into web pages for the Wistariahurst's website, and into Google Docs for use by its archivists.

Conclusion: Creating accessible data allows the people of Holyoke, MA to understand their history more. In conclusion, developing software that can clean and standardize data is valuable in all fields, especially for archival databases, where data must be organized for research. Data is generally quite messy, which produces issues of readability and understandability. By standardizing the data pipelines, we allow information to be easily translated between different applications and files. We are excited to continue working with the Wistariahurst Museum to further assist data management and cleanup during the fall semester.

Twisting Quantum Field Theories: Nilp Variety in the Orthosymplectic Super Lie Algebra

Chris Elliott[1], Ziji Zhou[1], Osha Jones[1]

[1]Department of Mathematics and Statistics, Amherst College, Amherst, MA, USA

Introduction: This project revolves around a mathematical approach to a physics topic of describing transformations in 3D space. Transformations called Lie Algebras and specifically the algebra osp(k|4,C) and important sub-spaces show an interesting triviality in translation or special conformal transformations as well as a way to describe the twist.

Methods: The work was centered around the nilpotence variety of osp(k|4,C) as well as the subspaces zQ and bQ, which are the kernel of even to odd morphism (zQ) and image of odd to even morphism (bQ) in osp. One specific element of Nilp of rank 2, Qx, was studied due to a presumption that it is representative of the family of rank 2 orbits. Computation with matrices and proving specific matrix representations and isomorphisms between special Lie Algebras. The process was also algorithmized to show the subspaces for all possible nilpotent elements.

Results: Two facts about the Nilpotence allowed us to fully describe this variety: All Q in Nilp have rank 1 or 2. Nilp is acted on by the Lie group G = SO(k, C) x SP(4, C) via conjugation, and zQ and bQ are preserved up to isomorphism within the orbits of G. As a consequence of these lemmas, we determined that there is one Nilp containing all rank 1 elements Q, and a family of orbits parametrized by x in C corresponding to all rank 2 elements Qx in Nilp. Additionally, the computations with Qx revealed that the twist, or the non-trivial transformations (or the quotient zQ/bQ), is isomorphic to the Lie Algebra so(k-4,C).

Conclusion: This project only touches a small area of a much larger field of study. One specific area of further exploration with more applicable physics implications is studying the orbits formed by the conjugation of the same group but over the Real field: G = SO(k, R) x SP(4, R). Additionally, generalizing this process for higher dimensions could likely reveal patterns that grant further insight.

Quantum q-Series Identities and Mock Theta Functions

Amanda Folsom[1], David Metacarpa[1], Wenche Tseng[1]

[1]Department of Mathematics and Statistics, Amherst College, Amherst, MA, USA

Introduction: The legacy of the mock theta functions, a collection of q-series (infinite basic hypergeometric series in the variable q) originally studied by Ramanujan c. 1920, persists today. Over the course of the last 100 years, they have been studied for their rich analytic and combinatorial properties, as key examples of mock modular forms in Analytic Number Theory, and for their connections to other areas of mathematics including Topology and Mathematical Physics.

Methods: Our research investigates the connections between mock theta functions and quantum modular forms via "quantum q-series identities," identities that do not hold between q-series within the complex unit disc but do at dense sets of roots of unity. We prove general quantum q-series identities that we apply to many different situations involving mock theta functions.

Results: We show that normalized limiting versions of two universal mock theta functions are quantum modular forms. We also find what we call "antiquantum q-series identities" for two third-order mock theta functions.

Conclusion: Via quantum q-series, we find new connections between mock theta functions and quantum modular forms.

Classification of Ideal Lattices of Leavitt Path Algebras

Ephrata Getachew[1], Yvan Grinspan[1], Emma Keenan[1], Alex Kupersmith[1], Seth Yoo[1]

Department of Mathematics and Statistics, Amherst College, Amherst, MA, USA

Introduction: A directed graph consists of a set of vertices and a set of edges connecting the vertices, with each edge assigned a direction. They can be used to represent networks of all types: social, economic, environmental, and informational. Directed graphs are often studied in the area of combinatorics, and they are relevant in computer science, physics and other STEM fields. Conveniently, directed graphs have an algebraic structure too. An algebra is a set with addition, multiplication and scalar multiplication.

Methods: We used tools from abstract algebra (rings and ideals), linear algebra (vector spaces and linear transformations) and graph theory (directed graphs, incidence and adjacency) to study the ideal structure of Leavitt path algebras for directed graphs.

Results: In this project, we focused on Leavitt path algebras and classified them up to isomorphism and ideal lattice equivalence for small graphs. We also provided a new graph theoretic proof of the characterization of graded ideals of Leavitt path algebras.

Conclusion: In conclusion, there is a correspondence between graph theory and algebra, via the ideal lattice structure of Leavitt path algebras of directed graphs. We characterized the equivalence classes of such algebras for small graphs (two vertices), and we described in terms of graph theory the difference between graded and non-graded ideals of Leavitt path algebras.

Subsystem CSS Codes over Prime Fields

Michael Liu[1], Victor Albert[1]

[1]Joint Center for Quantum Information and Computer Science, University of Maryland

Introduction: Quantum error correction is needed to mitigate noise in quantum computers. We study a particular class of quantum error correction protocols which have connections to classical coding theory.

Methods: In this work, we specialize further to a class of subsystem stabilizer codes which generalize subspace CSS codes [CS95]. Loosely speaking, we call H a subsystem CSS code if H admits a generating set in which each generator is a tensor product of only X Pauli operators or only Z Pauli operators.

Results: Immediately, one might ask whether subsystem CSS codes perform comparably to subsystem stabilizer codes, in terms of the number of physical, logical, and gauge qubits, as well as the code distance. We prove that this is indeed the case; any subsystem stabilizer code can be used to construct a subsystem CSS code with comparable code properties. Next, we discuss how the extra structure enjoyed by subsystem CSS codes allows a finer description of code properties such as structure and distance. In particular, we describe a special recovery procedure for subsystem CSS codes, which utilizes two classical linear codes to independently correct X type and Z type errors. Finally, we introduce general tools to study the structure of arbitrary subsystem stabilizer codes, and we define two generalizations of subsystem CSS codes which may be of further interest. Throughout, all vector spaces are assumed finite dimensional over a prime field F of characteristic p.

Conclusion: Potential applications to abelian anyon theories.

FLT3-L and TNF-α decrease suppressive capacity of human monocytic-MDSCs on T cell proliferation

Eugena Chang[1], Jennifer Wang[1], Stephanie Dougan[1, 2]

[1]Department of Cancer Immunology and Virology, Dana-Farber Cancer Institute, Boston, MA
[2]Department of Immunology, Harvard Medical School, Boston, MA

Introduction: This study investigates the impact of cytokines (FLT3-L, IL-18, and TNF-α) on the morphology and function of IL-6+GM-CSF-induced monocytic myeloid-derived suppressor cells (Mo-MDSCs) in vitro. Pancreatic ductal adenocarcinoma (PDAC) induces high rates of MDSC formation in both mice and humans. Tumor cells release cytokines and chemokines that induce high rates of myelopoiesis, resulting in immature myeloid cells being released into circulation. These myeloid cells are actively recruited into the tumor, where they differentiate into MDSCs, contributing to T cell suppression and malignant cell growth. In a recent clinical trial, PDAC patients received chemotherapy along with anti-IL-1β and anti-PD-1. Previous studies in mice had found IL-1β blockade in combination with chemotherapy or immunotherapy improved outcomes in tumor-bearing mice. This clinical trial found decreased myeloid suppression of peripheral CD8 T cells in patients on combination therapy. This study aimed to investigate the mechanism of IL-1β blockade in trial patients by inducing monocytes with various cytokines that increased following treatment to determine their effects on Mo-MDSC differentiation and function.

Methods: Monocytes and T cells were isolated from healthy human donor blood. Monocytes were cultured in healthy human serum, macrophage colony-stimulating factor, and various cytokines for 7 days. At day 7, differentiated monocytes were co-cultured with T cells. On day 3 of co-culture, T cell proliferation was measured using flow cytometry.

Results: IL-1β alone did not induce Mo-MDSC in vitro. When monocytes differentiated in Mo-MDSC-inducing cytokines (IL-6, GM-CSF) and 20ng/mL of FLT3-L or TNF-α, they did not have the suppressive capabilities of control Mo-MDSCs. CD8 T cell proliferation increased significantly with the addition of these cytokines. Monocytes cultured in 20ng/mL IL-18 alone suppressed CD8 T cell proliferation while other cytokines did not induce suppressive monocytes alone.

Conclusion: FLT3-L and TNF-α hinder the suppressive function of Mo-MDSCs in vitro. The reduced CD8 T cell suppression by patient-serum-induced monocytes following combination therapy may be partially due to the elevated levels of FLT3-L and TNF-α interfering with Mo-MDSC differentiation.

Quantification of Tissue Toxicity Post-Total Abdominal and Whole-Brain Irradiation Using Immunohistochemistry

Naviya Kapadia[1], Stavros Melemenidis[1], Suparna Dutt[1], Vignesh Viswanathan[1], Billy W. Loo Jr[1]

[1]Department of Radiation Oncology, Stanford University School of Medicine, Stanford, CA

Introduction: Radiation therapy is a common clinical treatment modality for many cancers. Healthy tissue damage as a result of irradiation (IR) is a significant side effect of treatment. The intestine and brain are highly radiosensitive. The current treatment standard—conventional dose rate (CONV) irradiation causes Lgr5+ cells such as CBCs to undergo apoptosis post-irradiation. CONV-IR also decreases hippocampal 5HT levels and disrupts hippocampal neurogenesis, leading to neurocognitive deficits, such as anxiety-like and depression-like behavior and impaired learning and memory.

Methods: To study and hopefully mitigate radiation-induced tissue toxicity, ultra-high dose rate FLASH-IR is applied to mouse models to draw a comparison between FLASH-IR and CONV-IR. Both total abdominal irradiation (TAI) and whole-brain irradiation were the focus of this study, with each treatment modality assigned one cohort of healthy mice. In mice that received TAI, cleaved caspase-3 staining on intestinal tissues quantified apoptotic CBCs in the intestine. New dosages for intestinal irradiation were explored—12 Gy versus the typical 14 Gy to reduce tissue toxicity. We also explored immunohistochemical (IHC) staining to replace the need for behavioral testing to determine cognitive deficits on mice post-whole-brain irradiation. On brain tissues, doublecortin (DCX) staining for hippocampal neurogenesis was performed. Cognitive effects of radiotherapy are thought to be due to hippocampal damage. By replacing behavioral testing with IHC staining, the time required to determine tissue toxicity is significantly lessened.

Results: We found a higher number of surviving CBCs in TAI-FLASH-IR mice compared to TAI-CONV-IR mice. More DCX positive hippocampal neurons appeared in whole-brain FLASH-IR mice compared to CONV-IR, however, final quantification of proliferating hippocampal neurons is not yet complete.

Conclusion: Our preliminary findings suggest FLASH-IR may lead to less tissue damage in highly radiosensitive tissues. When used in patients, ultra-high dose rate irradiation may reduce side effects that arise as a result of radiotherapy. TAI-FLASH may cause less gastrointestinal issues post-IR due to alleviation of tissue toxicity. In whole-brain irradiation, FLASH-IR may lead to less cognitive and behavioral deficits, as hippocampal neurogenesis appears to be spared. DCX staining highlighted proliferating hippocampal neurons, which may eliminate the need for behavioral testing post-IR. FLASH irradiation has potential to enhance patient comfort and become the new standard for efficient radiotherapy, starting at the deepest physiological level.

Additive Lifestyle Behaviors Mitigate MACE Risk: Mediated by Greater Reduction In Stress-Associated Neural Activity

Hannah Kim[1, 2], Taha Zafar Ahmad[1, 2], Natasha Savianu[1,2], Giovanni Civieri, MD[1], Shady Abohashem, MD[1], Ahmed Tawakol, MD[1]

[1]Cardiovascular Imaging Research Center, Massachusetts General Hospital, Boston, MA, USA
[2]Amherst College, Amherst, MA

Introduction: Lifestyle behaviors such as light/moderate alcohol consumption, healthy sleep and exercise have been individually associated with reducing MACE risk, via a mechanism involving reduced stress-related neural activity (SNA). However, their combined effect on MACE risk and SNA is unclear. We sought to evaluate the incremental effect of lifestyle behaviors on reducing MACE risk and SNA, and test whether SNA mediates this relationship.

Methods: Participants (from the Mass General Brigham Biobank) who completed a health behavior survey were studied between 2010 to 2020. A subset (N=629) underwent 18F-fluorodeoxyglucose positron emission tomography imaging enabling assessment of SNA as a ratio of amygdalar to ventromedial prefrontal cortical activity. Lifestyle score was composed of three behaviors: light/moderate alcohol consumption (0-14 drinks/week), sleep (7-9 hours/day), and exercise (500 METs/week). MACE was determined based on international classification codes of disease 10th edition (ICD-10). Covariates were evaluated based on ICD-10 codes and health survey data. Linear and cox regression models were employed.

Results: Of the 53,068 participants (median age 59 years, 51% women), 42,462 had low/moderate alcohol consumption, 29,713 slept 7-9 hours/day, and 35,335 exercised 500MET/week. Over a median follow-up of 3 years, 26,731 experienced MACE. Greater lifestyle score associated with decreased SNA (standardizedβ [95% confidence interval (95%CI)] = -0.105 [-0.183, -0.027], p=0.009) and lower MACE risk (Hazard Ratio (HR) [95%CI] = 0.842 [0.805, 0.881], p<0.001) after adjusting for age, gender, and cardiovascular risk factors. Each additional lifestyle behavior (LB) incrementally lowered MACE risk (LB1: Hazard Ratio (HR) [95%CI]: 0.780 [0.707, 0.861], p<0.001; LB2: HR: 0.658 [0.597, 0.725], p<0.001; LB3: HR: 0.530 [0.477, 0.588], p<0.001).
In a mediation analysis, SNA significantly mediated the effect of lifestyle behaviors on reducing MACE risk, accounting for 6% of this relationship (Total indirect Effect [95%CI]: -0.0197 [-0.0478, -0.0010]; p<0.05).

Conclusion: Lifestyle behavior incrementally decreases MACE risk and SNA. Reduced SNA mediates the link between lifestyle behaviors and MACE risk, accounting for 6% of this relationship. Future randomized trials should investigate the potential of a combined lifestyle approach on reducing SNA and MACE risk.

Discovering new links between pesticide exposure and Parkinson's Disease

Alexia Lapadat[1], Brittany Krzyzanowski[1], and Brad A. Racette[1]

[1]Racette Laboratory, Neuroepidemiology Research Program, Barrow Neurological Institute, St. Joseph's Hospital and Medical Center, Phoenix, AZ

Introduction: Parkinson's disease is the fastest-growing neurological disorder in the world. In the past decades, a widely discussed risk factor has concerned environmental contaminants, notably pesticide exposure. There is growing concern about the lack of regulation for agricultural chemicals, leading to numerous campaigns to ban pesticides such as paraquat. This study aims to uncover the pesticides with the strongest association with Parkinson's Disease (PD) in the USA.

Methods: We conducted a population-based geographical study of Medicare beneficiaries (aged 67+) in 3064 U.S. counties, using a dataset of 450+ pesticides obtained from annual estimates of agricultural pesticide application provided by the United States Geological Survey. We modeled nationwide association maps for the 65 pesticides with sufficient data using MGWR, an advanced spatial regression software. In this study, we computed the 95% confidence intervals (CI) and retained only the statically significant counties.

Results: We identified a region in the Rocky Mountains/Great Plains where the association between several pesticides and PD was strongest. We did a deeper exploration of the top 14 pesticides of interest using linear regression modeling, and we found that lindane, simazine, and atrazine had the strongest relationships with PD. Furthermore, we also confirmed previously investigated associations of chlorpyrifos and paraquat with PD. This study identified several other promising understudied pesticides (thifensulfuron, metalaxyl) associated with PD.

Conclusion: In our society, we are exposed to various chemicals whose toxicities and health risks we do not fully understand yet. Our findings reflect the growing need for meticulous regulations and bans on pesticides.

Antithrombotic Therapies for Patients Following Endovenous Recanalization

Rina Li[1, 2], Andrea Sarafolean, RN[2], Ellen Cravero, MS[2], Nedaa Skeik, MD[3]

[1]Department of Sociology, Amherst College, Amherst, MA, USA
[2]Minneapolis Heart Institute Foundation, Minneapolis, MN, USA
[3]Vascular Medicine, Minneapolis Heart Institute, Minneapolis, MN, USA

Introduction: Deep vein thrombosis (DVT) is a subtype of venous thromboembolism and has serious sequelae of post-thrombotic syndrome and pulmonary embolism. In cases of severe DVT, interventional radiology techniques are considered. This study aims to assess the effectiveness and safety of three antithrombotic therapy options in patients following iliocaval recanalization.

Methods: A retrospective cohort study of 128 patients at Abbott Northwestern Hospital in Minneapolis, Minnesota with iliocaval venous obstruction or thrombosis requiring thrombolysis and/or thrombectomy with or without venoplasty/stenting between 2010 and 2023.

Results: The combination of antiplatelet and anticoagulant therapy was associated with higher vein patency ($p=0.3$), lower recurrent thrombosis ($p=0.10$), and lower bleeding rates ($p=0.5$) at the first follow-up visit than anticoagulant or antiplatelet alone. However, the differences were not statistically significant.

Conclusion: This single-centered study provides insight on post-procedural antithrombotic therapies following endovenous recanalization. Larger studies are needed to confirm and expand on the observed trends.

Comparison of Surgical Outcomes Between Endoscopic and Open Reconstructive Approaches in Treating Metopic Synostosis

Frances Lin[1], Ariel Figueroa, MD[2], Kareem Termanini, MD[2], Taylor Hallman, BS[2]; Alice Yau, BS[2], Marina Lentskevich, BS[2]; Arun K. Gosain, MD[2]

[1]Amherst College, Amherst, MA, USA
[2]Ann & Robert H. Lurie Children's Hospital, Chicago, IL, USA

Introduction: Infant skull plates are connected by flexible joints called cranial sutures that provide flexibility for vaginal birth and rapid brain growth. Metopic synostosis is a condition where the metopic suture fuses prematurely, resulting in a triangular head shape and midline ridge across the forehead. Open cranial vault reconstruction has traditionally been used to correct the abnormal head shape, but there is increased interest in treating the condition with an endoscopic strip craniectomy and orthotic helmet. An endoscopic strip craniectomy possesses a better safety profile and comparable cosmetic satisfaction. However, limited comparisons of the quantitative surgical outcomes and small sample sizes along with the absence of standard morphological parameters in metopic synostosis have made it difficult to conclude whether endoscopic strip craniectomies are objectively comparable to open reconstructions. Therefore, this study analyzed a larger and growing cohort's quantitative outcomes between the two treatments to validate and expand upon existing findings using recently published craniometrics.

Methods: This retrospective study compared various quantitative outcomes between open cranial vault surgery and endoscopic strip craniectomy in treating metopic synostosis. Measurements included the diagonal frontal angle, cranial index, and anterior-posterior width ratios collected from patients' pre-operative and post-operative light scans.

Results: Open reconstruction led to a greater increase in the frontal angle and anterior-posterior width ratios than an endoscopic strip craniectomy. However, there was no significant difference in the post-operative cranial index between the two treatments.

Conclusion: Open reconstruction and an endoscopic strip craniectomy effectively reduced forehead narrowing with the former resulting in a greater increase in the frontal angle. Open reconstruction also demonstrated a greater increase in the anterior-posterior width ratios, which suggests it may better normalize head shape but differences in patient age between treatment groups may account for differences in skull growth. Overall, it remains unclear if one surgical approach is superior due to the lack of patients who underwent an endoscopic strip craniectomy. The study is ongoing and will continue to collect patient data to generate a more robust analysis of the surgical outcomes.

Using Lasso Regression to Select Important Electrodes in a Brain-Computer Interface

Alexandra Olson[1], Cody Watson[2], Albert Wilson[3]

[1]Amherst College, Amherst, MA, USA
[2]Northwestern University, Evanston, IL, USA
[3]Georgia State University, Atlanta, GA, USA

Introduction: Brain Computer Interfaces (BCIs) allow individuals to communicate without moving their bodies and are critical for patients with ALS and NMDs. The P300 BCI design uses a 16-channel electrode cap and a visual flashing letter grid to communicate a message. Mental counting of the target flash of a desired letter initiates an event-related potential, a P300 peak, in the user's EEG. The electrode cap records EEG data from 16 channels, and a prediction model uses the data from all channels to predict the target letter. Using 16 channels results in longer set-up times, greater financial cost, and variance in the time of the EEG signal. This project's goal was to select significant electrodes and reduce the number of channels without greatly compromising BCI classification accuracy.

Methods: A Lasso Regression model was trained and individually fitted for 10 participants aged 18-26. Since each channel is associated with 26 time points (and thus 26 coefficients in the prediction model), Lasso reduced non-important coefficients for each channel to 0. Channels were ranked from 1 to 16 within each participant based on their proportion of significant (non-zero) predictors, and their ranking was averaged across all 10 participants. A permutation test on the mean channel ranking determined which channels were statistically significant ($p < 0.05$). The significant channels from all 10 participants were combined to create a generalized model. Using only the subset of universally important channels, character accuracy was re-tested on 29 total participants and compared to character accuracy prior to feature selection.

Results: Lasso Regression selected 5 important electrodes overall. 24/29 (83%) of the participants experienced a character accuracy reduction no greater than 10% even when 11 channels were removed. 15/29 (51%) of participants even had 0% change in accuracy or experienced an accuracy improvement. An analysis of the 5/29 (17%) of poor-performing participants with greater than a 10% accuracy reduction revealed they were all in the middle-age range (31-59) and 3 of them had ALS. Differences in model quality between ALS and non-ALS participants were not statistically significant ($p = 0.18$).

Conclusion: Lasso Regression was able to reduce the 16 electrode model to just 5 electrodes. 3 of these electrodes were located in the occipital lobe and were found to be the most significant. The occipital lobe has a vital role in processing visual information and tracking rapid flashes in the BCI. Reducing the BCI from 16 electrodes to 5 electrodes would save up to $20,000 per device and reduce time during BCI set-up while still maintaining reasonable accuracy.

Deep Convolutional Neural Network to Estimate Cardiovascular Disease Risk from Chest Computed Tomography

Daniel Oo[1, 2], Vineet K. Raghu, PhD[2], Audra Sturniolo, MS[2], Michael T. Lu, MD, MPH[2]

[1]Department of Mathematics and Statistics, Amherst College, Amherst, MA, USA
[2]Cardiovascular Imaging Research Center, Massachusetts General Hospital, Boston, MA, USA

Introduction: Primary prevention of atherosclerotic cardiovascular disease (ASCVD) is dependent on accurate risk estimation. Current risk estimation models use patient information found in the electronic medical record. However, there is information in chest computed tomography (CT) images beyond typical risk factors that contributes to risk estimation. We test whether deep convolutional neural networks can extract these features from chest CT to improve estimation of ASCVD risk.

Methods: We developed a deep learning model (CT-CV-Risk) using 51,182 lung cancer screening chest CTs from 12,433 participants in the National Lung Screening Trial. The CT-CV-Risk model was trained to predict cardiovascular mortality over 12 years of follow-up. Independent testing was performed using only a single baseline CT from a held-out set of 7,405 individuals with no history of type 2 diabetes, myocardial infarction, or stroke (i.e. eligible for primary prevention) for the prediction of 12-year cardiovascular mortality. Results are provided in the testing dataset only. CT-CV-Risk was compared to a baseline regression model using demographics, smoking, BMI, and comorbidities.

Results: In the independent testing dataset of 7,405 persons (mean age 61.0 ± 4.9 years; 65.9% male), 3.4% of individuals died of cardiovascular disease. Adding the CT-CV-Risk score to the baseline regression model significantly improved discrimination for cardiovascular mortality (combined C-index 0.72 [0.69, 0.75] vs. baseline C-index 0.69 [0.66, 0.73], $p < 0.001$). Similar results were seen for a secondary outcome of fatal myocardial infarction (combined C-index 0.72 [0.67, 0.77] vs. baseline C-index 0.69 [0.64, 0.74], $p < 0.001$).

Conclusion: Based on a single chest CT, CT-CV-Risk predicted 12-year cardiovascular mortality beyond prevalent risk factors. We demonstrate that deep learning can estimate cardiovascular risk from a chest CT image. This may enable opportunistic risk assessment using existing CTs to help guide primary cardiovascular prevention.

tdTomato-STOP: A Versatile Reporter for Detecting Genome Editing

Alexander L. Yan[1, 2], Samuel W. Du[1, 3], Krzysztof Palczewski[1, 3, 4, 5]

[1]Center for Translational Vision Research, Department of Ophthalmology, University of California, Irvine, Irvine, CA
[2]Neuroscience Program, Amherst College, Amherst, MA
[3]Department of Physiology and Biophysics, University of California, Irvine, Irvine, CA
[4] Department of Chemistry, University of California, Irvine, Irvine, CA
[5]Department of Molecular Biology and Biochemistry, University of California, Irvine, Irvine, CA

Introduction: Adenine base editors (ABEs) and prime editors (PEs) are CRISPR/Cas9 derived agents that enable precise DNA edits that can correct many of the pathogenic mutations causative of genetic diseases. ABEs and PEs are highly programmable to target a specific genomic locus by their respective single guide RNAs (sgRNAs) and prime editor guide RNAs (pegRNAs). However, the safety profile and efficiency of genome editor delivery must be further developed to minimize deleterious off-target editing. Common approaches to screening novel delivery methods involve experiments in mammalian cells, which often require laborious and resource-intensive processing to assess editing outcomes. In contrast, a fluorescence-based assay in mammalian cells can provide rapid and straightforward screening of genome editing.

Methods: We designed a construct encoding the fluorescent protein tdTomato harboring two C>T mutations that introduce stop codons (TAG) into each monomer, which was named tdTomato-STOP. Correction of these mutations by ABE or PE would allow readthrough and restored expression of tdTomato. After preliminary verification of the editing construct, a lentivirus packaging the tdTomato-STOP construct was produced and used to transduce HEK-293T cells, stably integrating the tdTomato-STOP gene into the HEK 293T genome. After antibiotic selection, a clone stably expressing tdTomato-STOP was selected based on favorable characteristics such as editing efficiency, growth kinetics, and morphology.

Results: We delivered ABE as plasmid, mRNA, and ribonucleoprotein to the tdTomato-STOP cells, which achieved robust restoration of tdTomato expression as assessed by microscopy and flow cytometry. Further, on-target genomic modifications were confirmed by amplification of the target sequence and subsequent Sanger sequencing. Finally, we identified several pegRNAs with the highest efficiency and lowest ratio of unintended edits and off-target effects, which can be used for future tdTomato-STOP experiments.

Conclusion: We have established a fluorescence-based tool to sensitively detect ABE and PE activity in cells, which verifies on-target genome editing without the need for DNA sequencing or Western blot. tdTomato-STOP can thus be widely utilized for safety and efficiency studies of novel genome editor delivery technologies in vitro, from viruses to lipid nanoparticles.

Endotoxin-Sequestering Nanoparticle Protein Coronas to Mitigate Inflammation in Cancer

Ryan Yim[1], Jacob Shaw[2], Ryan M. Pearson[2, 3]

[1]Nathan Schnaper Intern Program in Translational Cancer Research, Baltimore, MD, USA
[2]Department of Microbiology and Immunology, University of Maryland, Baltimore, MD, USA
[3]Department of Pharmaceutical Sciences, University of Maryland, Baltimore, MD, USA

Introduction: Cancer patients are more susceptible to sepsis-related immune complications due to their immunocompromised condition. Amongst cancer patients, 3.7% of patients are diagnosed with sepsis and sepsis-related mortality accounts for 9% of cancer deaths annually. Lipopolysaccharide (LPS) is an endotoxin that originates from Gram-negative bacteria cell walls and plays an important role in the pathogenicity of sepsis by inappropriately signaling host innate immune responses, systemic organ damage, and death. Immune cells produce an abundance of antimicrobial biomolecules, such as cytokines, defensins, antimicrobial peptides, and proteins, to aid in clearing the infection and sequestering/inhibiting LPS; however, this often proves to be insufficient. Poly(lactic-co-glycolic acid) (PLGA) nanoparticles (NPs) have been frequently employed as drug delivery agents for chemotherapeutics. Moreover, the Pearson Lab has demonstrated the particles are inherently anti-inflammatory using in vitro and in vivo models of endotoxemia. Although these NPs mitigated the exaggerated innate immune response, they did not directly combat bacterial infection or circulating LPS. Proteomics analysis revealed composition of plasma proteins that interact with the NPs to form a protein corona, a layer of adsorbed proteins, on the surfaces of NPs. Lactoferrin (Lf), an antimicrobial and anti-LPS protein, was identified as highly abundant. This research examines the utilization of Lf as a precoating to form an anti-inflammatory protein corona on the PLGA NPs.

Methods: PLGA NPs were incubated with different concentrations of Lf and assessed through DLS, SDS Page, and BCA Assay. ELISA's were carried out for immunogenic analysis, followed by FITC-LPS experimentation for endotoxin sequestration under different solvent conditions.

Results: Lf bound to the NP surface in a concentration-dependent manner and Lf content was between 1% to 30% of the total NP weight. Lf-coated NPs were non-immunogenic when assessed using bone marrow-derived macrophages. Lf-coated NPs demonstrated a 30% release of Lf over a 42 hour time point. A trend towards significance was observed in LPS sequestration in the presence of fetal bovine serum (FBS).

Conclusion: Lf is demonstrated to bind abundantly to the PLGA NPs. Passive release of Lf as a precoating shows strong potential and will require further sequestration experimentation specifically to LPS. Further analysis is needed under the condition of FBS and FITC-LPS, specifically at different concentrations of either NPs, Lf, or FBS.

Once upon a mechanosensation: Zyxin recruitment to dynamic neuronal structures

Ramapriya Balagurunath[1], Nisan Sele[1, 2], Braxton R. Schuldt[1, 3], Sally A. Kim[1].

[1]Amherst College, Department of Biology & Neuroscience Program,
[2]University of Massachusetts Amherst, Psychology & Brain Sciences,
[3]Nash Family Department of Neuroscience, Icahn School of Medicine at Mount Sinai

Introduction: Cells are able to sense mechanical cues and transduce these signals into intracellular responses through the process of mechanosensation. In muscle cells, tension forces on stress fibers induce zyxin localization to F-actin to regulate changes in the cytoskeleton. The key player in this process is zyxin, a focal adhesion protein that plays a crucial role in remodeling F-actin but has yet to be described in the central nervous system— specifically in neurons.

Methods: Here, we characterize the mechanosensitive nature of zyxin in rat hippocampal neurons (Days In Vitro (DIV) 13-15), focusing on the dynamic subcellular compartments of dendrites and spines, the excitatory postsynaptic (receiving) sites for neuronal signals. Through live cell imaging, we found that mechanical stress increased eGFP-zyxin localization to both dendrites and spines in neurons. To identify this part of the mechanosensitive pathway in hippocampal neurons, we inhibited the phosphorylation of myosin II using Y27632 (ROCKi), a ROCK inhibitor.

Results: We found that under ROCKi conditions, average fluorescence intensity at the spines remained stable throughout imaging, indicating that changes in eGFP-zyxin localization were blocked by the drug. This finding implicates zyxin as mechanosensitive in neuronal spines and dendrites. Furthermore, we found that the spine area under control conditions increased throughout imaging but remained stable under ROCKi conditions; this suggests a connection between zyxin translocation and changes in spine shape.

Conclusion: These findings demonstrate the potential role of zyxin in dendritic growth, spine maturation, and synaptic plasticity. Understanding the mechanoregulation behind these processes in the brain may also provide insight into the molecular mechanisms underlying neurodegenerative and neurodevelopmental conditions.

Par-1 Overexpression Does Not Affect Bruchpilot Localization in Drosophila

Tate Eppinger[1], John P. Roche[1]

[1]Department of Neuroscience, Amherst College, Amherst, MA

Introduction: MARK/Par-1 is a kinase that is thought to regulate protein transport in synapses. Par-1 is present in both humans and in the model organism Drosophila melanogaster (fruit fly). MARK/Par-1 misregulation has been connected to neurodegenerative disorders and autism spectrum disorders. Furthermore, MARK/Par-1, as well as the closely related MARK2, MARK3, and MARK4, can all phosphorylate or hyperphosphorylate Tau. This is connected to Alzheimer's disease. In this study, we overexpressed Par-1 presynaptically in Drosophila and examined its effects on Bruchpilot, an important and well-studied presynaptic protein.

Methods: We overexpressed Par-1 in an experimental group of flies using a Gal4/UAS system. Gal4 is a gene that encodes the yeast transcription activator protein Gal4, which can bind to a UAS sequence to activate upstream transcription if present. Both flies with overexpressed Par-1 and a wildtype control group were dissected, fixed with 4% paraformaldehyde, and stained using fluorescence antibodies. Primary antibodies of m-α-BRP and rb-α-GluRC were added in concentrations of 1:250 and 1:2500, respectively. Secondary antibodies of Cy3-α-mouse, A488-α-rabbit, and Cy5-α-HRP were all added at 1:1000. Images were taken on muscle 4 synapses using a confocal microscope at 63x magnification. Analysis was performed on Fiji image analysis software. Intensity was measured in a highlighted area by the mean gray value of the pixels. Apposition data was collected by counting the number of BRP and unopposed GluRC puncta.

Results: The results of this study indicate no significant change in BRP localization with Par-1 overexpression (Par-1OE). Intensity in both synapses and axons was unchanged between WT and Par-1OE ($p>0.05$, $p>0.05$). Apposition between BRP and GluRC was also unchanged ($p>0.05$).

Conclusion: In this report we show that presynaptic overexpression of Par-1 does not affect the localization of a well-studied presynaptic protein, Bruchpilot, in Drosophila. Although overexpression of Par-1 did not affect BRP in muscle 4, further studies are possible to determine Par-1's effect on BRP in other locations in Drosophila. Par-1 should also be investigated for its potential effects on other presynaptic proteins.

Layer-specific analysis of mu-opioidergic & pain-responsive cells in the mouse and rhesus macaque anterior cingulate cortex (ACC)

Sofi Farinas[1], Jacqueline W. K. Wu[1], Lisa M. Wooldridge[1], Nora M. McCall[1], Gregory J. Salimando[1], & Gregory Corder[1]

[1]Department of Neuroscience, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA

Introduction: An estimated 20% of US adults experience chronic pain. While opioid analgesics remain widely used for severe pain, they can produce detrimental side-effects including addiction and respiratory depression. Thus, an ideal analgesic that avoids side-effects might target select pain-processing, opioidergic cell populations outside of the brain's canonical reward or homeostatic regulatory centers. A key brain area with dense MOR expression is the anterior cingulate cortex (ACC), which has been implicated in encoding the negative emotional experience of pain. However, little is known about the specific ACC cell-types expressing MOR that encode pain, whether certain ACC sub-regions are more involved in pain processing than others, and if cortical architecture is conserved across species.

Methods: To address this, we used immunohistochemistry and in situ hybridization to conduct layer-specific analyses of both MOR+ and pain-responsive cells in mouse and rhesus macaque ACC.

Results: Here, we report that the expression of MOR is found across all parts of ACC but enriched in deeper cortical layers in mouse and macaque tissue. Additionally, we find that pain-responsive cell-types in mice are distributed across all parts of the ACC but are enriched in the deeper layers as well. Lastly, we report on the use of a novel viral approach to gain genetic access within MOR+ cell-types in mouse and macaque ACC and validate the specificity of viral transgene expression against endogenous MOR expression.

Conclusion: Together, our layer-specific analysis and new viral tool present a targeted way to selectively engage these same cortical populations for future study and manipulation.

MEF2C knockout induces innervation defects in L2/3 neurons

Luis E. Guzmán Clavel[1, 2], Sriram Sudarsanam[1], and Alex L. Kolodkin, PhD[1]

[1]Solomon H. Snyder Neuroscience Department, The Johns Hopkins School of Medicine, Baltimore, MD, USA
[2]Department of Neuroscience, Amherst College, Amherst, MA, USA

Introduction: The cortex relies on the precise targeting of axonal projections to organize complex neuronal circuits. For example, layer II/III (L2/3) neurons in the primary somatosensory cortex (S1) innervate L2/3 and L5 targets both ipsi- and contralaterally, in addition to forming precise long-range connections. The disruption of these circuits underlies several neurodevelopmental disorders, such as ASD, schizophrenia, and epilepsy, often after the loss of function of area-specific transcription factors (TF). Here, we describe how Mef2C, a L2/3 enriched TF, regulates the formation of area-specific connectivity of primary somatosensory (S1) L2/3 neurons in the murine cortex.

Methods: Using temporally controlled in utero electroporation (IUE) of a construct expressing Cre recombinase in Mef2c floxed mice allowed the deletion of Mef2C specifically in S1 L2/3 neurons. This was combined with bulk and sparse neuronal labeling approaches involving co-electroporation of Cre-dependent fluorescent reporter constructs. This allowed us to study the connectivity of L2/3 neurons locally in the ipsilateral S1, and distally, in the long-range innervation targets of these neurons.

Results: WT S1 L2/3 neurons stereotypically project their axons through the white matter to homotypic cortical areas, where they form innervation columns. Ipsilaterally, primary targets include the border between S1 and secondary somatosensory cortex (S1/S2 border), the primary motor cortex (iM1), and local innervation through layer-specific collaterals in L2/3 and L5. Contralaterally, L2/3 neurons cM1, cS1/cS2 and separately to S2. Additionally, they also project to both insular cortices (iIC, cIC). Mef2c cKO S1 L2/3 neurons displayed severe deficits in long-range connectivity. cS1/S2 border and cS2 innervation columns were completely abolished, and there was a significant deficit in the midline crossing of Mef2c CKO axons. At other long-range cortical targets such as the iS2 and insular cortices, axons from Mef2c CKO neurons did not project to the more superficial laminae. Finally, local axonal-collateral deficits were observed.

Conclusion: These findings suggest that Mef2C is a critical regulator of the connectivity signature of L2/3 neurons, and its loss of function severely impairs the development of proper axonal projections to canonical targets. These include the loss of long-range area-specific projections, as well as the disruption of local layer-specific circuits. Altogether, our results point towards the need for Mef2C in the development of the precise connectivity patterns of cortical L2/3 neurons, whose disruption underlies several neurodevelopmental disorders.

The Effect of Sec8 on Exosomal Vesicle Release in Drosophila Neurons

Chris Halada[1], John P. Roche[1]

[1]Department of Neuroscience, Amherst College, Amherst, MA, USA

Introduction: Sec8 is a protein involved in the exocyst protein complex, a group of proteins that have multiple functions in various cells. While there are many known functions of the exocyst as it acts throughout the cell, further research is required to understand its function in neurons as well as what protein components of the exocyst complex are necessary for certain cellular functions. Neuromuscular junctions are complex cellular environments where vesicle release is critical to synaptic function, plasticity, and elongation. One type of vesicle release that has been associated with the exocyst complex is the release of exosomal vesicles. Thus, researching Sec8's role in the exosomal vesicle release will provide a better understanding of the overall function of the exocyst in neurons and determine whether sec8 is a critical component involved in this process. Previous research has found that the exocyst subunit sec15 mediates neuronal targeting and function as well as the release of vesicular exosomes in neurons. Here we would like to determine if other exocyst subunits contribute to the release of exosomal vesicles.

Methods: Three wildtype Drosophila third instar larva (control) and three UAS Sec8 RNAi larva were dissected in ice cold phosphate buffer solution (PBS) and then fixed in a 4% paraformaldehyde solution. After being washed and treated in a normal goat serum block, the larvae were treated overnight at 4° C with m−α-BRP 1:250, rb−α-DGluRIII 1:2500, and α-NRG 1:200 primary antibodies. The larvae were then washed in PBS+ Triton and then treated with secondary antibodies at 1:1000 for 45 minutes. The larvae were incubated in glycerol for an hour before being mounted to a glass slide. The slides were viewed through a confocal microscope and z-stack images of the stained NMJs were taken using a 63x objective lens. Images were analyzed using FIJI software. The integrated density (ID) of the NRG channel for the NMJ was subtracted from the ID of the NRG channel for the NMJ scaled 1.5x to determine the post synaptic levels of NRG, a known component of the exosomal vesicles.

Results: Due to multiple experimental errors while mounting larva, I was only able to gather data on 5 larva. If I was able to gather sufficient data on both control and experimental groups, I would be able to compare levels of exosomal release by quantifying the postsynaptic Nrg levels in both the control and experimental groups. Our hypothesis was that Sec8 is crucial for exosomal vesicle release. If Sec8 is crucial for vesicular exosomal release, we would expect to see significantly lower postsynaptic NRG levels than seen for the experimental group larvae.

Conclusion: Due to a lack of data on Sec8 RNAi larva, we are unable to draw any conclusions about the effects of the RNAi on exosomal vesicle release. For future experiments I would be more diligent in handling the treated larvae and increase the sample size. This experiment could also be replicated with other proteins that may be involved with vesicle release. with vesicle Release.

Pre-Adolescent Sex Differences Exist in Relative Amygdala Subnuclei Size

J. Max Landa[1, 2], L. Nate Overholtzer[3, 4], Megan M Herting[3]

[1]Dept. of Biology, Amherst College, Amherst, MA.
[2]NGP Neural Summer Program, University of Southern California, Los Angeles, CA.
[3]Dept. of Population and Public Health Science, Keck School of Medicine of USC, Los Angeles, CA.
[4]USC-Caltech MD-PhD Program, Keck School of Medicine of USC, Los Angeles, CA.

Introduction: This study investigates sex differences in amygdala composition, a subcortical limbic system structure. We aimed to characterize subnuclei volumes in a large sample of pre-adolescent male and female children across a narrow age range. Additionally, our goal was to explore late childhood sex-related differences in relative subnuclei volumes as a fraction of total hemispheric amygdala volume.

Methods: Using the in vivo CIT168 probabilistic atlas, we visually segmented and quantified 9 subnuclei regions of the amygdala. We compared the probabilistic volume (PV) and relative volume fraction (RVF) of each subnuclei across both sexes using independent T-tests.

Results: We observed high-quality segmentation results of amygdala subnuclei in subjects that met the CNR threshold. Most subjects displayed minimal to no overlap of individual subnuclei at a 0.5 threshold during visual quality control. FDR-corrected T-tests showed significant bi-hemispheric RVF differences in the Central Nucleus (CEN), left hemispheric differences in the Cortical and medical nuclei (CMN) and Amygdala Transition Area (ATA), and right hemispheric differences in the Amygdalostriatal Transition Area (ASTA).

Conclusion: The CIT168 probabilistic atlas provided a high-quality segmentation of amygdala subnuclei in a large, diverse sample of pre-adolescent children ages 9-10 years old. Our sample also provides evidence of pre-adolescent sex differences in amygdala subnuclei morphometry.

Cellular Pathophysiology of the Hippocampal Dentate Gyrus in a Mouse Model of Dravet Syndrome

Hasun Noh[1], Amishi Mahajan[2], Yerahm Hong[2], Amelia J. Eisch[1, 3], Sanghee Yun[1, 3]

[1]Dept. Anesthesiology Critical Care Med, Children's Hospital of Philadelphia, Philadelphia, PA
[2]University of Pennsylvania, Philadelphia, PA
[3]Dept. Anesthesiology Critical Care Med, Perelman School Med Univ. Pennsylvania, Philadelphia, PA

Introduction: Dravet Syndrome (DS) is a treatment-resistant genetic epilepsy disorder, which is caused by a mutation in the SCN1A gene, which consequently results in brain hyperactivity, causing seizures. Pediatric DS patients have neurodevelopmental disabilities, including decreased learning and memory. Hyperactivity reaches its peak during the chronic epileptic stage, but prior studies have not done DG subregional analysis during this stage. The goal of this study was to quantify proliferating cells in the dentate gyrus of a SCN1A+/- mouse model and its WT littermates with specific focus on the number of proliferating cells in two categories: those that typically give rise to new neurons (subgranular zone [SGZ]), and those that do not (outer granule cell layer [oGCl], molecular layer [ML], and hilus). We hypothesized that relative to their WT littermates, SCN1A+/- mice would have more SGZ proliferating cells as well as ectopic proliferation in oGCL, ML, and hilus.

Methods: 11-week-old SCN1A+/- mice and WT littermates were given bromodeoxyuridine (BrdU, 150mg/kg, i.p.), a thymidine analog, to label proliferating cells in the S-phase of the cell cycle two hours prior to perfusion and after a series of behavioral tests. Brain sections were processed for slide-mounted immunohistochemistry with a BrdU antibody. BrdU immunoreactive (BrdU+) cells were counted via unbiased stereology.

Results: Male and female adult SCN1A+/- mice had a significantly higher number of BrdU+ proliferating cells in the SGZ than their WT counterparts. Further investigation into ectopic proliferation show that female SCN1A+/- mice had a significantly increased number of BrdU+ cells in the ML, oGCL, and hilus than female WT mice (Cohen's-d ≥ 0.50). In male SCN1A+/- mice, the number of BrdU+ cells was similar in the hilus and oGCL between SCN1A+/- and WT mice, but displayed a decreased amount of proliferating BrdU+ cells in the ML.

Conclusion: These data suggest that at the time of BrdU injection, the DG of female SCN1A+/- mice was hyperactive vs. WT mice. While no evidence of hyperactivity was found in male mice, the experimental design and relatively low subject number prevent us from concluding that this is a sex-specific result. Future experiments are warranted to increase subject number, directly compare sex differences, and quantify different genres of proliferating cells. The present data urge closer consideration of DG region-specific seizure-induced proliferation in developing DG-targeted interventions and treatments for DS.

The Relationship between Zebrafish Larvae Age and Startle Response Latency

Ahmad Ziada[1], Stacey Beganny[1], Josef G. Trapani[1]

[1]Department of Biology, Amherst College, Amherst, MA, USA

Introduction: This research project investigates the relationship between the age of zebrafish larvae and the latency of startle response. The startle response is a defensive behavior that enables animals to escape threats such as predator strikes. Examining zebrafish startle and comparing the latencies across zebrafish between 5 and 8 days post fertilization (dpf), the project aims to provide some insight into the relationship between early developmental age and this important response.

Methods: The project used optogenetics, a research technique that controls neuronal activity using light and genetic engineering. In the zebrafish line used in the experiments (myo6b:ChR2-EYFP), Channelrhodopsin-2 (ChR-2) is a light-gated, non-specific cation channel protein that is expressed in the hair cells of the ear and lateral line. Zebrafish were screened for the expression of ChR-2 by identifying YFP (fluorophore that is tagged to ChR2 in this transgenic line) fluorescent neuromasts in the lateral line and ear using a Nikon SMZ1500 microscope and a SOLA light source. Five ChR-2-expressing larvae were chosen from each age (5,6,7,8 dpf), and each larva was stimulated five times while free-swimming (waiting 2 minutes between each stimulus to prevent habituation). The stimulation was done by placing a larva in a RODI water droplet in a petri dish and placing the dish in a recording chamber under an LED light source that shined blue light (470 nm) for 50 ms. SutterPatch software was used to create an experiment routine to deliver a consistently timed, voltage-based command across all experiments. The zebrafish response was then recorded using a high-speed camera (xiQ MQ013MG-ON) at 500 fps. The videos were collected for each zebrafish and analyzed manually for the difference in time between the light and startle response onsets.

Results: The results indicate an impact of age on the latency of the startle response. The mean latency across the four age groups was different, but without any clear trend observed (25.04 ± 8.02 ms, 22.72 ± 7.23 ms, 26.30 ± 11.28 ms, and 26.43 ± 10.50 ms at 5,6,7,8 dpf, respectively). It was also observed that with age, the values of the latencies became more dispersed.

Conclusion: In conclusion, age seemed to impact the latency of the zebrafish startle response, but without a clear trend. It also appeared to affect the distribution of the startle response latencies, making them more dispersed. The experiment can be improved by increasing the camera's frame rate since more accurate latency values can help determine the type of the startle response. Also, measuring the light intensity will give more insight into the latency values obtained.

Cosmic Blueprints: Unraveling the Architecture of Planet-Forming Disks

Josie Carrillo[1], Kate Follette[1], Cat Sarosi[1]

[1]Amherst College, Amherst, MA, USA

Introduction: This research paper investigates planet-forming disks at different wavelengths visually. By examining their shape and morphology at different wavelengths to gain insight on the disk as one whole. In turn we can investigate the relationship of these shapes and learn more about the planet formation process.

Methods: This project build's upon Cat Sarosi's previous goal to quantitatively and visually describe the morphology and properties of a planet-forming disk. Four planet-forming disks will be imaged at different wavelengths and converted into RGB images to visually display overlapping features. This will be used to study potential correlations of the disks at different wavelengths as well as be implemented into a Python class.

Results: The results of this project produced a function that images clear RGB images. The function can take in user input to affect qualities such as the zoom, brightness, and coloring. It automatically centers the disks at different wavelengths and highlights the overlapping disks by recoloring them. This function is plays an integral part in being able to simplify the characterization of planet-forming disks visually.

Conclusion: In conclusion, this work provides a substantial step forward in being able to characterize planet-forming disks. These results can in turn prove useful to understanding the early process of planet formation.

Constraining Beyond the Standard Model Sub-MeV Neutrino Fluxes Using the XENONnT Detector

Noah Chavez[1], Amy Flather[2], Ian M. Shoemaker[3]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA
[2]Rutgers University, Piscataway, NJ, USA
[3]Center for Neutrino Physics, Virginia Tech University, Blacksburg, VA, USA

Introduction: This work uses experimental data from dark matter direct detection experiments to apply model-independent neutrino flux constraints to previously unconstrained regions of the Grand Unified Neutrino Spectrum. Since some beyond the standard model (BSM) phenomena like decaying dark matter and decaying primordial black holes predict a low-energy neutrino flux, this work is a step towards ruling out certain models of BSM physics.

Methods: Using recently published data from the XENONnT dark matter direct detection experiment, this work employs a maximum log-likelihood method in combination with a model comparison test to obtain flux constraints. This work compares the experimental data from the XENON collaboration to predicted data that would arise from a hypothetical neutrino flux. It is then possible to determine whether the hypothetical neutrino flux is valid.

Results: This work extracts the first sub-MeV model-independent neutrino flux bounds. We place flux constraints of 10E5 (cm^2 s eV)^-1 at a 90% confidence level for neutrino energies from 16keV to 1.8MeV. These constraints explore neutrino energies an order of magnitude lower than the previous lowest constraints, set by the Borexino experiment. Although the constraints this work obtains are not strong enough to eliminate any models of BSM physics, this work is a step toward validating models of new physics. Moreover, these findings demonstrate the feasibility of using dark matter direct detection experiments to obtain low-energy model-independent neutrino flux constraints.

Conclusion: In summary, this work obtains model-independent neutrino flux constraints in the previously unexplored sub-MeV energy range using experimental data from dark matter detectors provided by the XENON collaboration. By setting these constraints, we demonstrate that dark matter detectors can apply neutrino flux constraints at extraordinarily low energies. Furthermore, this work motivates the creation of future dark matter detectors with greater exposure and efficiency as a tool for both dark matter physics and neutrino physics.

Determining Dynamical Masses and Orbital Parameters of M-Dwarf Companions

Henry Dennen[1], Piper Lentz[1], Alec Treadway[1], Daniella Bardalez Gagliuffi[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst MA, USA

Introduction: As part of an ongoing effort to categorize celestial objects within 20 parsecs, we investigated the companions of M-dwarfs, the coldest and lowest mass stars. By examining the companions of M-dwarf primary stars, we hope to contribute information that will prove beneficial in discerning the formation mechanisms of brown dwarfs, and celestial bodies on the line between stars and planets.

Methods: Using proper motion accelerations from Gaia and Hipparcos astrometry, and radial velocity from existing literature, we can construct a 3D motion model of the companion's motion. Importing this data into a Python program, orvara, and using a Markov Chain Monte Carlo (MCMC) to randomize orbital parameters and dynamical mass, we determine orbital parameters and dynamical masses of the target's companion.

Results: We determined precise dynamical masses of the companions to 2 M-dwarfs and 1 hotter solar-type star for comparison. We determined the brown dwarf companion G239-25B to have a dynamical mass of 0759 ± 3.5 m⊙, and constrained its orbital parameters. Additionally, we found Ross690b, a super Jupiter exoplanet with a dynamical mass of .0037 ± .0003 m⊙. However, we were able to fit two solutions for the inclination of its orbit, indicating a solution for retrograde and prograde orbital motion. Finally, we examined HD24916B, an M2 binary star companion with a dynamical mass of .522 ± .04 m⊙. We were not able to arrive at a single, well-constrained solution to its eccentricity, so more investigation is needed.

Conclusion: Categorizing a variety of companions with vastly different mass ratios is a promising step forward in identifying systems that will allow us to investigate formation mechanisms. Most companion masses are based on models, so using radial velocity and astrometry in tandem to determine precise dynamical masses helps to flesh out existing catalogs of companions.

Fixing the Bucket Angle on a Centrifugal Force Microscope

Jai Dreher[1], Audrey Orlowski[1], Gigi Golden[1], Ashley Carter[1]

[1]Amherst College, Amherst, MA, USA

Introduction: With a Centrifugal Force Microscope (CFM), we can view the unfolding of DNA by protamine, a process made easier if the buckets within the CFM are held at a constant 45 degree angle (maximizing the force on the DNA). Thus, the goal of this project is to design and build a piece that can withstand rotational forces and balance issues, all while holding the buckets at that constant angle.

Methods: Top down construction in SolidWorks (3D CAD) was used on an existing CFM bucket structure, allowing for the utilization of existing geometry. The designed piece was then printed in plastic and tested in the centrifuge.

Results: The piece attached successfully to all buckets with no need to force the parts to fit. Further, the CFM ran smoothly with the piece incorporated at 300 then 500 rpm. Upon opening, the structures were fully intact and functional.

Conclusion: Now having a working prototype of the piece in plastic, the next steps will be to construct the piece out of metal, a much more durable option. As of now however, we can conclude that the prototype works as designed, holding the buckets at the constant 45 degree angle, and withstanding significant rotational forces.

Probing Glassy Behavior in Antiferromagnets

Melanie Huq[1], Soho Shim[2], Kannan Lu[2], Greg MacDougall[2], Nadya Mason[2]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA
[2]Materials Research Laboratory, University of Illinois, Urbana-Champaign, IL, USA

Introduction: Our research studies antiferromagnets, a magnetic material whose internal magnetic moments cancel each other out. Antiferromagnets are good candidates for spintronics, which seeks to use magnetism to make faster and more efficient devices. Iron niobium sulfide is an antiferromagnet that also contains spin glass, regions where magnetic moments freeze below a certain temperature. Furthermore, iron niobium sulfide can rapidly switch its spins' orientations and displays anisotropic magnetoresistance (AMR), where its resistance is influenced by the magnitude and orientation of a magnetic field. These properties make iron niobium sulfide especially interesting for spintronics. However, we must better understand the interactions between iron niobium sulfide's antiferromagnetic and spin glass regions to understand its full potential. Here, we examine if the AMR of iron niobium sulfide is affected by its spin glass regions.

Methods: We designed devices made of iron niobium sulfide flakes connected to six gold leads. For each device, we used a magnetic field to orient its spin glass in different orientations, a process known as field-cooling. After each field-cooling, we measured the flake's AMR by measuring its resistance while varying the angle between the flake and an external magnetic field.

Results: We found that in some samples, the AMR of iron niobium sulfide changes depending on the angle of the magnetic field used in field-cooling. This suggests that the spin glass regions interact with the material's antiferromagnetic regions, causing changes in AMR based on the spin glass' orientation. However, other samples lack this dependence, implying that iron niobium sulfide samples have varying amounts of spin glass.

Conclusion: Our research examined how the spin glass and antiferromagnetic regions in iron niobium sulfide interacted. While we found that spin glass orientation could affect iron niobium sulfide's AMR, we also found that one flake had no spin glass. These findings demonstrate that AMR can be an effective tool to identify spin glass in materials, due to clear differences in AMR in flakes with and without spin glass. Our work has also helped quantify the properties of iron niobium sulfide, potentially contributing to the development of faster, more efficient technology.

Benign Beam Behavior in the Battle for Better Boson Bounds

Andrew Glassford[1], Saif Salim[1], Dr. Nathan Clayburn[1], Professor Larry Hunter[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: Many Standard Model extensions predict novel forces and bosons (including axions, paraphotons, dark photons – dark matter candidates!). We look for long-range, spin-dependent forces with a Hg-Cs co-magnetometer. Spin-dependent forces modify the potential energy difference between magnetic sublevels of the Hg ground state, changing its spin precession frequency from just what the ambient magnetic field should produce. Using Earth as a spin-polarized source, we rotate our apparatus with respect to Earth's surface and look for changes in precession frequency. Our signal units are thus microhertz of Hg spin-precession frequency (Hg μHz). We measured a statistically significant signal in May and need to investigate its source.

Methods: We procured a quadrant detector that reacts to position as a function of beam radius. By holding our laser steady and walking the detector at known intervals, we were able to calibrate the detector and get the radius of our beams as a bonus. We then rotated our apparatus between its four available positions and measured the amount of wander in each laser beam.
Next, we procured a motorized mirror mount to precisely control our beams. After using the position detector to calibrate the mirror mount, we walked the lasers ±300 microns from the center while taking measurements of our Hg-Cs co-magnetometer signal. We then reran the walking-measuring procedure several times with different voltages on our auxiliary ("gradient") quadrupole magnetic field coils to see how changes in the magnetic field gradient affect the signal's sensitivity to motion.

Results: We measured the worst beam motion to be 60 microns at the detector, which corresponds to 30 microns at our vapor cells. Because the vapor cells contain the Hg and Cs samples, we assume they account for variations in our signal and work in terms of movement at the cell.
We found a specific voltage for our gradient coils that should minimize the signal sensitivity to beam motion to zero at around 5.4 V ± 0.26V. Combining the uncertainty in the correction voltage, the slope of sensitivity-to-motion versus voltage, and worst beam wander, we were able to bound the effects of beam motion to 0.011 Hg μHz, well below our stated sensitivity goal of 0.07 Hg μHz.

Conclusion: While we failed to explain our anomalous signal, we did successfully characterize the effect of beam wander and found it to be well within our tolerance. Towards the end of the summer, we noticed that the outer magnetic shield was bumping into the main shaft of the apparatus. Given how sensitive the atoms are to fluctuations in magnetic field, and how reactive the shields are to pressure and stress, we suspect this may be our answer. We have begun the process of investigating the shield effects. We will continue to investigate potential sources of error until we exhaust every option.

Growth of germanium from solid Ge using halide vapor phase epitaxy

Megan Goh[1], Edgard W. da Costa[2], Kevin Schulte[2], John Simon[2], Aaron Ptak[2]

[1]Amherst College, Amherst, Ma
[2]National Renewable Energy Lab, Golden, Co

Introduction: III-V solar cells are the most efficient solar cell but are extremely expensive to produce. Halide vapor phase epitaxy (HVPE) is a deposition technique that could potentially reduce costs by utilizing less expensive precursor materials and materials and by having a significantly faster growth rate when compared to the most common methods of III-V growth. We study the growth of germanium (Ge) from a solid Ge source by HVPE. Ge is a component of some high efficiency solar cells, and its growth can be used to re-use Ge substrates.

Methods: We use the HVPE reactor to grow Ge samples at different growth conditions. We measure film thickness using specular reflection measurements and model the data to determine the growth rate of each layer. We also used several microscope techniques to study the surface morphology, including Nomarski optical microscopy, atomic force microscopy (AFM), and scanning electron microscopy (SEM).

Results: We performed growth at pressures between 150 and 550 Torr and observed higher growth rates, but also surface roughness, for higher pressures. The growth rate also increased with growth temperature from 650 and 825°C. We calculate an activation energy of 8.8 kJ/mol for the Ge growth reaction at 350 torr. We find that the addition of arsine and phosphine to the Ge growth drastically increases the growth rate to up to 107.57 ± 0.04 nm/min, which indicates that the addition of active hydrogen is a key to increasing deposition rates when using a solid Ge source.

Conclusion: We grew Ge from a solid Ge precursor using HVPE. We showed how different parameters in our growth reactor affected Ge growth, and we found that adding hydrides to the reaction greatly increased our growth rates by bringing active hydrogen to the surface. In the future, we will work to make a smoother surface as well as work to optimize the growth rate.

Fractional Vortex Creation in Bose-Einstein Condensation at Low Field

Kateryna Havryshchuk[1], Dineth Wijayawardana[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA USA

Introduction: Over the summer, our group worked on developing fractional vortices in the Bose-Einstein Condensation (BEC) at low field. Our research explores a particular type of topological excitations in the BEC and has the potential to solve mysteries of superfluids, superconductors, neutron stars, and even quantum computers.

Methods: Often referred to as the fifth state of matter, the Bose-Einstein Condensate (BEC) appears from the cloud of Rb-87 atoms cooled down to almost an absolute zero and highly condensed. Due to the BEC rules, the quantum state of atoms throughout the condensate must either remain the same or change gradually. This property explains why the BEC is the appropriate environment for creating quantum vortices. While the state changes only once around the vortex in the singly-quantized structures, sometimes such structures break into less energetic half- and third-quantized vortices (i.e., fractional), which are characterized by the half- and third-quantum rotation of the state around the vortex core. Such vortices can be developed by inducing the singly-quantized vortices in the spinor-2 condensate and letting this structure evolve in time.

Results: This summer, our team succeeded in creating half-quantized vortices in the biaxial nematic magnetic phase of the condensate. We did it in the relatively low magnetic field, finally proving the spinor nature of such vortices. We also improved the technology for analyzing fractional vortices and set the foundation for inducing third-quantized vortices in the cyclic-tetrahedral phase in the fall.

Conclusion: We concluded that fractional vortices in the Bose-Einstein Condensate can be developed and analyzed. By using the low field, we proved the spinor nature of the vortices we observed and dispelled doubts about the possibility of their creation in the lab settings. While having succeeded with half-quantized vortices, we still need to improve the state preparation technology to create third-quantized vortices in the future.

Quantum Communications in Optical Fibers

Freddy Herrera Cueva[1], Prem Kumar[1], Gamze Gul[1]

[1]Center for Photonic Communication and Computing, Electrical and Computer Engineering Department, Northwestern University, Evanston, IL, USA

Introduction: Quantum communications is a fundamental building block for the development of a future quantum internet. A quantum internet would enable quantum teleportation, distributed quantum computing, and other advanced quantum technologies that could revolutionize information processing, making it possible to perform tasks that are currently impossible or extremely time-consuming. Our long-term goal is to build a robust quantum information network where the quantum payload is wrapped by classical header bits that help us monitor and control the network with classical telecom protocols.

Methods: Sources of entangled photon pairs based on spontaneous parametric processes are widely used in quantum information experiments. Our efforts are aimed at characterizing and optimizing the nonlinear effects of two-photon interference (TPI) in communication systems. More concretely, we study the generation of multiple pairs of polarization-entangled photons on the visibility and coincidence-to-accidental ratio (CAR) measurements. For this purpose, we use optical fibers as a medium that can transmit photons efficiently over long distances with minimal loss and noise, which is essential to preserve the delicate states of qubits.

Results: At the theoretical level, we are able to find an explicit dependence of the visibility and CAR factors on the average photon pair number, collection efficiencies of our detectors, and dark counts. Experimentally, however, our measurements of both communication factors did not agree with the predictions of our multiple-pair model. One possible explanation is that our current model is too idealistic and does not take into account other nonlinear processes that may be occurring in our setup, such as spontaneous Raman scattering and birefringence in our periodically polished lithium niobate (PPLN) crystal.

Conclusion: In conclusion, we are still in the initial stage of our long-term Quantum Wrapper Networking (QWN) research project. We are currently working on expanding our model and considering the effects of the above mentioned nonlinear optical phenomena. Additionally, to date, all our experiments have been based on purely quantum states in the O-band. Our next step is to study the coexistence of quantum and classical information in both the C-band and O-band within the same network.

Identifying Correlations in Precessing Gravitational-Wave Signals with Machine Learning

Karen Kang[1], Simona Miller[2], Katerina Chatziioannou[2], Deborah L. Ferguson[3]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA
[2]Department of Physics, California Institute of Technology, Pasadena, California, USA
[3]Center for Gravitational Physics and Department of Physics, The University of Texas at Austin, Austin, TX USA

Introduction: Binary binary hole (BBH) spins provide unique and important insights into the formation environments, evolutionary history, and dynamics of these objects. We would like to gain a better understanding of merger-dominated signals for highly massive highly spinning BBH systems, which are prone to spurious measurements due to their very short duration and low bandwidth. Astrophysical parameters from gravitational wave (GW) sources are extracted by match-filtering signals with numerical relativity (NR) waveforms templates. The degeneracies in waveforms, where dissimilar parameters yield similar waveforms, further complicates source identification. Using machine learning, we can visualize these degeneracies in the 7-dimensional BBH parameter space and develop models to quantify parameter correlations.

Methods: We developed an algorithm of mapping out the waveform parameter space, spanning all mass and spin dimensions, of BBHs iteratively: the algorithm evaluates the local covariance with respect to the reference injection, then proceeds to identify the next point of reference until boundary is reached. The choice of subsequent injections is based on the degenerate region's principal eigenvector, statistically modeled by Bayesian Gaussian fitting and Principal Component Analysis (PCA). When the dimensions are insufficient to fully characterize the BBH, we add in a K-Nearest Neighbor (KNN) approximation in selection.

Results: We verified correlation recovery accuracy of our algorithm in the effective spin (χeff)-symmetric mass ratio (η) space, where a linear degeneracy is well established. We mapped out the 4-D parameter space of aligned spin components (a1z, a2z), effective spin (χeff), and mass ratio (q), and overplotted the traced path on the transformed plane χeff - η plane. The plotted path and the χeff-η parameter space are in agreement .

Conclusion: A motivating event for this study is GW190521, which is the the heaviest BH binary detected to date and notably one of the few BBHs measured to be highly precessing. As precession effects remain elusive in the merger-dominated waveform, our future work would be dedicated to deciphering the complexities of BBH precession parameters. Spin configurations are indicative of the compact progenitor's orbital dynamics and therefore help illuminate the formation channels of BH mergers in the pair-instability (PI) mass gap and aid population modeling. Ultimately, we aim for an analytical model for spin parameters from simulations.

Fitting Orbits and Determining Dynamical Masses of Exoplanets within 20 Parsecs

Piper Lentz[1], Daniella Bardalez Gagliuffi[1], Henry Dennen[1], Alec Treadway[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: The movement of a star in both the plane of the sky and toward and away from Earth allows us to predict the orbital and dynamical parameters of a celestial companion, such as an exoplanet, brown dwarf (a "failed" star), or another star. Our research focused on predicting the orbital and dynamical parameters of systems within 20 parsecs to help build a comprehensive model of companion formation.

Methods: We gathered Gaia and Hipparcos acceleration data along with ground telescope radial velocity measurements of target stars to give us a three-dimensional motion model of the target stars, which we then imported into a Python code called Orvara. Orvara fits random samples of the orbital parameters and mass of our companions and calculates the probability that those random fits reflect the system parameters we imported.

Results: For the target star 20CrtA, a K-dwarf, the companion was determined to be a brown dwarf with a dynamical mass of about 74 Jupiter masses. For the target star HD131977, a K-dwarf, the companion was determined to be an exoplanet with a dynamical mass of about 6.5 Jupiter masses. For the target star HD110315, a K-dwarf, the companion was determined to be an M-dwarf star with a dynamical mass of about 245 Jupiter masses.

Conclusion: Our research is background work, we analyze systems within 20 parsecs. If we find a unique system, the James Webb Space Telescope may take a closer look to see how the companion was formed. Once we know how several systems formed, we can start constructing a model of companion formation. With this model, we could predict how newly found companions were formed, and if they are comparable to Earth or other planets that may support life.

Measuring Quantum Properties of Borosilicate Glass

Jeremiah Levy[1], Jonathan Friedman[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: This poster studies the quantum properties (most notably ones relating to anisotropy of spin-1 systems) of Borosilicate glass, that make it a candidate for quantum computing/information research. Deducing specifically the values of the longitudinal anisotropy constant D, allows us to understand the qualities of Borosilicate glass that give it a clock transition (one of the key components that make up a good qubit).

Methods: Using both an ACMS and cryostat to cool the sample down to 1.8 K, data will be collected on the magnetization of the sample when moved up rapidly through a set of detection coils at a steady field. Data will be analyzed within MatLab utilizing the EasySpin package, both to run simulations for a sample with the same characteristics, and fit our data to expected results to derive anisotropy constants.

Results: The signal created from the paramagnetism of the spins in a magnetic field is read as a magnetization (field strength) of those spins. Magnetization data was plotted against the Field from 0 to 9 Tesla, for eight distinct temperatures ranging from 1.8 to 20 K. Taking that data and scaling it along the x-axis (plotting field over temp for the x-axis) indicates that anisotropy is present within the data, as when plotted as a function of B/T, not all temperatures fall along the same curve. Using EasySpin to fit the data returns values of g = 3.85 and D = 84600 MHz, D being the objective of this experiment, the longitudinal anisotropy constant.

Conclusion: Given that the sample showed not only paramagnetic behavior but also was able to be fitted by the simulation for magnetometry on borosilicate, this implies that the given values of g and D are trustworthy for this experiment. Currently we believe clock transitions to be caused by the Boron within the glass, however further testing is necessary to confirm that theory. ACMS data collection on Soda Lime glass samples, aluminosilicate and AGC40 samples is currently being done, to compare with the borosilicate trials, and see if they have similar anisotropy. Aluminosilicate has a similar chemical makeup to Borosilicate.

Probing Substellar Formation with Spectra of Low Mass Brown Dwarfs and Stars

Bethany Martin[1], Amy Zheng[1], Prof. Kate Follette[1], Jada Louison[2]

[1]Amherst College
[2]University of Massachusetts, Amherst

Introduction: Accretion is the process of an object gaining matter by attracting surrounding dust and gas along its magnetic field lines. When in-falling material shocks at its surface, the object emits excess ultraviolet and optical emission which can be analyzed with spectroscopy to infer the object's mass accretion rate. This project examines the excess continuum at shorter wavelengths of accreting low mass brown dwarfs and stars to infer mass accretion rates and better understand the formation of substellar objects (brown dwarfs and planets).

Methods: For this project, we focus on brown dwarfs, substellar objects with masses ranging from 13-75 Jupiter masses, as well as very low mass stars. We use data from two datasets obtained from the Keck Low-resolution Imaging Spectrometer (LRIS) atop Mauna Kea, HI. These are the Herczeg 2006 study and a June 2021 observation run. To obtain our calibrated spectra, we use PypeIt, a Python software package for spectroscopic extraction.

Results: We produce blue-side (shorter wavelength) flux-calibrated spectra for eight young, low mass brown dwarfs and four low mass stars. The resulting flux-calibrated spectra show that the accreting brown dwarfs have more excess continuum emission over the non-accreting template, which indicates the objects are still gaining mass. In addition, accreting objects have a noticeable Balmer jump in which the flux drastically decreases near 360 nanometers.

Conclusion: In conclusion, this project shows that these objects are continuing to gain mass through accretion and we can examine their formation processes through spectroscopy. This will allow for further study of substellar formation processes and the differences between brown dwarf and low mass star formation paradigms. Additionally, once the spectra undergo post-reduction steps, mass accretion rates can be inferred.

Search for widely separated companions for WISE 0830+2837, A Step Towards Understanding Y-Dwarf Binary Systems

Klara Matuszewska[1], Daniella Bardalez Gagliuffi[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: This project aims to analyze new images from the James Webb Space Telescope (JWST) to identify potential companions to WISE 0830+2837 (W0830), the second coolest brown dwarf known. Existing in the Y-dwarf category, W0830 lies at the intersection between stars and gas giant exoplanets. We set specific criteria for identifying companion sources: they should be fainter, redder, and a comover to the primary brown dwarf target. Then, using these constraints we identified candidates for individual analysis.

Methods: Initially we constructed a color-magnitude diagram (CMD) in order to identify all objects fainter than our target. Determining an object's brightness (absolute magnitude) however requires knowknowledge of the distance to each object. Since most of the sources visible in the new JWST images are being seen for the very first time, we had no information on their distances. We therefore assumed all sources to be at the distance of W0830 since a potential candidate would be.

After establishing the fainter candidates through the CMD, we proceeded to investigate their colors. This was executed by computing the difference in flux between the two JWST filters: 150W (bluer) and 480M (redder). A positive value indicates that a source is redder, meaning it is brighter in the 480M filter and fainter in the 150W filter. This color comparison aided in isolating sources that meet the "redder" criterion.

The final characteristic we investigated was whether a source is a comover with the primary brown dwarf target, W0830. Due to the limitation of having JWST images from only one epoch, we supplemented with an older Spitzer image from 2019. While the time gap between the Spitzer and JWST images was just three years, most objects remained approximately stationary in the sky. However, W0830 has high proper motion so there was a clear difference in its position. This allowed us to identify sources that exhibited similar motion to W0830 over this time.

Results: The sensitivity of JWST revealed numerous new sources, and while when assuming to be at the same distance as the target they all turned out to be fainter, only two of them were found to be redder.
- Candidate 1: Although seeming redder, it was overly bright in the 150W filter, disqualifying it.
- Candidate 2: This candidate was absent in the 150W images, keeping it viable based on color. However, it did not share W0830's proper motion and was therefore disqualified.

Conclusion: After our analysis, we confirmed W0830 as a solitary Y-dwarf brown dwarf, with no companions satisfying all established criteria. The study highlights W0830's unique status in the Y-dwarf category and showcases the power and limitations of the James Webb Space Telescope in identifying new celestial objects.

The Creation and Observation of Three-Dimensional Skyrmions in Spin-2 Bose-Einstein Condensates (BECs)

Isla Steinman[1]

[1]Department of Physics and Astronomy, Amherst College, Amherst, MA, USA

Introduction: This summer, I attempted to create and photograph a three-dimensional topological excitation known as a skyrmion that occurs in BECs in particular magnetic phases subject to a particular magnetic field configuration. A BEC is a superfluid state of matter that forms when dilute bosonic gases are billionths of a degree above absolute zero and when their atoms are in their lowest energy state or ground state. Our BECs were made of Rubidium 87 which has two hyperfine energy levels within the ground state. BECs with atoms in various states in the hyperfine energy level, F, is known as a spin-F BEC. We study BECs because they are macroscopic but exhibit behavior identical to quantum phenomena that is more difficult to observe. Thus, we can gain insights in quantum phenomena without having to work with microscopic quantum matter. We particularly study topological excitations because they have applications in quantum computing, astrophysics, and cosmology.

Topological excitations are structures that cannot be deformed continuously, for example, a Möbius Strip. The Möbius Strip cannot form a ring because it has a twist in it that cannot be undone unless the strip is cut, untwisted, and then glued back together. A skyrmion is a three-dimensional topological excitation we make in our BECs.

We make skyrmions in BECs that can be described by a magnetic phase at every point. The magnetic phase can be represented as a shape known as a spherical harmonic. If you alter the orientation of the spherical harmonic, you can alter the shape of the BEC. To make the skyrmion, we create the initial magnetic phase, then imprint the skyrmion in the BEC. The two magnetic phases we used to make skyrmions were biaxial nematic and cyclic-tetrahedral. To imprint the skyrmion, the orientation of the spherical harmonic must change continuously in particular ways throughout the entire condensate.

Methods: We use microwave pulses to create the initial magnetic phase—biaxial nematic or cyclic-tetrahedral—in the BEC. Then, we imprint the skyrmion in the BEC by rapidly changing the apparatus' magnetic field from a uniform field to a quadrupole shape and placing the zero of the field at the center of the condensate for 0.5 milliseconds winding the full skyrmion.

Results: After many adjustments to the initial magnetic phase preparation and the apparatus' magnetic field, we successfully created and imaged fully wound biaxial nematic and cyclic-tetrahedral skyrmions in our BECs. These skyrmions are more complicated than those that have been previously observed.

Conclusion: Using biaxial nematic and cyclic-tetrahedral phases, we successfully magnetically imprinted fully wound skyrmions in spin-2 BECs. This summer, we took the clearest images of these skyrmions to date.

Psychology

Exploring Metacognitive ability in preschoolers' elective trust

Vaughn Armour[1], Carrie Palmquist[1]

[1]Department of Psychology, Amherst College, Amherst, MA, USA

Introduction: This study asked 4 and 5-year-olds to weigh different kinds of cues to make decisions in a standard selective trust task. We also explored whether individual differences in metacognition, need for cognition, and theory of mind predicted how children evaluated different pieces of information in the trust task.

Methods: This study underwent four trials of an epistemic trust task, which were conducted on a computer. We also ran a test of Metacognitive ability with three different knowledge scenarios. We then did Theory of Mind test on a computer, with six different Theory of Mind scenarios increasing in difficulty. The final part was a fourteen question Need For Cognition survey. All of these questions were about how kids thought, with seven of them focused on seeking knowledge, and four of them focused on conquering it.

Results: The results of this study indicate that males ($p = .022$) and those who choose to learn more about the subject's knowledge of other objects ($p = .043$) ask the "correct" person for help more often. Children who ask for more pieces of information endorse the "correct" person more often ($p = .038$). We also found that children chose three different strategies for solving the trust task: picking one piece of information every time, picking three pieces every time, and switching between strategies. Kids who always picked one were more likely to be male($p <.001$), lower in NFC conquer ($p =.005$), and younger ($p <.001$). Those who picked three every time were more confident ($p = .011$), lower in theory of mind ($p = .014$), higher in NFC Conquer ($p < .001$), and younger ($p= .003$). Kids who switched were older ($p < .001$), less confident ($p = .002$), higher in theory of mind ($p = .029$) and chose to learn about the subject's knowledge of other objects earlier ($p < .001$).

Conclusion: Our initial question was whether children were explicitly aware that some pieces of information about others may be more helpful in determining whether they will be a good source of information or not. They were not, but they did differ in how they attacked that information. Younger kids tended to choose one strategy and stick with it, while older kids switched between strategies. We found that kids answered ask and endorse similarly, but their developmental differences governed their information-seeking paths.

Exploring Children's Trust in Learning From ChatGPT

Ada Chen[1], Justin Ruiz[1], Carrie Palmquist[1]

[1]Department of Psychology, Amherst College, Amherst, MA, USA

Introduction: As children increasingly interact with new technology, it is important to know how children perceive different sources of information. With age and advancing reading skills, children rapidly come to regard written text as a dominant source of information. Children between the ages of 4-8 begin to see the internet as a reliable source of scientific and historical information (Wnag et. al., 2019). Previous research has found that children prefer seeking factual information from voice assistants over human informants. This research paper explores children's unknown perceptions of new AI software that emulates a hybrid between written text and voice assistance. We ask the following questions: (a) How confident are children in ChatGPT's pedagogical capacity? (b) What are children's preferences of sources across different domains of information? (c) What attributions and prior experiences influence their perceptions and evaluations of each source?

Methods: This study will analyze data collected from a total of 40 participants at the age of 10. Our preliminary sample contains 30 participants, 14 girls and 16 boys. Participants were led through four different trials; Induction, Endorse, Ask, and Attribution. Induction familiarized participants with each of the three sources (ChatGPT, written text, human). Participants were asked if the informant was "correct or incorrect" and gave a subsequent confidence rating in the Endorse Trials. In the Ask trials, children were asked to rank the the informnats from most to least reliable for questions categorized under three domains (stable, transient, personal). Attribution Trials consisted of yes/no questions pertaining to participants attributions of each source.

Results: Results from the Ask trials indicate that a preferred source exists across all three domains of questions. The first choice rankings were statistically significant across all three domains. Children preferred written text sources for stable questions, ChatGPT for transient questions, and the human source for personal questions. When asked transient and personal questions children explicitly ranked sources from most to least reliable, indicating that children are generating assumptions on the limitations and possibilities of differing sources. No patterns were present in how confident and likely children are to endorse information from different sources.

Conclusion: In conclusion, this study provides evidence that children perceive ChatGPT as a new entity that is versatile. This study also provides the foundation for future research comparing children's trust in ChatGPT directly to voice assistants. In addition, a replication can model how trust in differing sources changes overtime as the usage of AI as an educational tool increases.

Insecure Attachment Styles in Romantic Relationships and Emotion Regulation

Chéla Cunningham[1], Elizabeth Kneeland[1], Mabel Shanahan[1]

[1]Amherst College, Amherst, MA, USA

Introduction: This study investigates the relationship between insecure attachment styles in romantic relationships and mental health. By examining emotion regulation strategies, relationship satisfaction, anxiety, and depression, the study aims to emphasize the importance of identifying unhealthy attachments and understanding their impact on relationships.

Methods: This study will analyze data collected through a self-reported survey administered on Prolific. The survey will assess emotion regulation strategies, relationship satisfaction, and attachment to one's romantic partner, as part of a larger study examining humor and emotion beliefs, in addition to attachment style. The study aims to explore the potential effects on romantic relationships.

Results: The results of this study indicate statistically significant negative effects of insecure attachment on romantic relationships. Analysis of survey data revealed a significant decrease in relationship satisfaction ($p < 0.001$) and a significant increase in negative interactions ($p < 0.05$) when participants indicated they had insecure attachment styles. Similarly, those with insecure attachment also indicated employing more maladaptive emotion regulation strategies such as self-blame ($p < 0.05$) compared to those with secure attachment styles. The findings highlight the potential harm of unaddressed insecure attachment, particularly within romantic relationships, emphasizing the urgency of recognizing and addressing attachment patterns for healthier and more fulfilling interpersonal connections.

Conclusion: In conclusion, this study highlights how detrimental insecure attachment styles can be to relationships. These attachment styles are linked to higher levels of depression, decreased relationship satisfaction, and a greater tendency to use maladaptive emotion regulation strategies. These findings highlight the importance of considering attachment styles, particularly during times of conflict in couples.

Laughter is the Best Medicine? The Implications of Self-Enhancing Humor in Emotional Sensitivity, Loneliness, and Depression

Alexandra S. Hollin[1], Elizabeth T. Kneeland[1], & Mabel Shanahan[1]

[1]Department of Psychology, Amherst College, Amherst, MA, USA

Introduction: The current study examined humor as a coping mechanism and the effects of positive humor styles on emotion regulation and mental wellbeing. We hypothesized that individuals reporting high usage of positive humor styles would be more successful at emotion regulation and would report fewer feelings of loneliness and depression than individuals that report high usage of negative humor styles. We also aimed to explore loneliness and emotional sensitivity as mediators between humor styles and depression.

Methods: Participants completed a series of self-report questionnaires to assess humor styles, emotion regulation strategies, emotion reactivity, loneliness, and mental health.

Results: Use of self-enhancing humor had a significant negative correlation with levels of loneliness, emotional sensitivity, and self-blame and a significant positive correlation with levels of positive refocusing. Loneliness and emotional sensitivity mediated the negative correlation between self-enhancing humor and depression.

Conclusion: Higher use of self-enhancing humor was positively correlated with use of positive emotion regulation strategies and increased wellbeing. These results suggest that self-enhancing humor may allow individuals to reappraise difficult situations and unpleasant emotions to be more positive. Future research could further explore the impact of negative humor on wellbeing and use a larger sample to help determine stronger significance.

Evaluating the Effect of Psychiatric Comorbidity on Development Using Healthy Brain Network Data

Jude O. Ighovoyivwi[1, 2], Torre Lloyd[3]

[1]Columbia University Mailman School of Public Health, New York, NY, USA
[2]Amherst College, Amherst, MA, USA
[3]Winston-Salem State University, Winston-Salem, NC, USA

Introduction: Psychiatric Comorbidity is the presence of two or more mental disorders in one individual. As individuals mature, demographic variables such as age, sex, ethnicity, and language, can influence what type/pattern of psychiatric comorbidities they might develop overtime.The primary objective of this study is to identify psychiatric comorbidity patterns in children and adolescents and find an association with subjective and objective developmental outcomes.

Methods: This study analyzes data collected by the NKI-RS between 2013 and 2017 as a resource to accelerate scientific understanding of brain development and disruptions associated with the onset of psychiatric illness. 455 participants will be included in the study sample. We will study the effect of socio-demographic variables such as sex (Male/Female), age, and Ethnicity on the pattern of comorbidities participants might develop as they mature. We will focus primarily on ADHD, as well as other psychiatric Disorders such as OCD and Separation Anxiety Disorder. Using poLCA packages in R studio, we will create an LCA (Latent Class Analysis) regression model to determine the number of latent classes (clusters) that would estimate the lowest Bayesian information criterion (BIC) and best quantify how well our clusters explain the variance in our data. After identifying the number of clusters that would provide the lowest BIC, we will conduct cluster analysis to illustrate what diagnoses show significant differences across clusters, and how our socio-economic variables can explain these differences.

Results: The results of this study showed that age was the primary factor behind the diagnosis prevalence across the different clusters. Specifically, we observed that younger children tended to have ADHD comorbid with ticks, while older children, primarily found in our third cluster, were more likely to have inattentive subtypes with internalized disorders. Regarding sex differences, we did not observe significant variations between the psychiatric groups in terms of gender distribution. However, overall, males tended to have a higher prevalence of psychiatric disorders because ADHD was the main contributing factor, and ADHD is generally more common in males.

Conclusion: In summary, this study offers compelling evidence suggesting that children diagnosed with ADHD have an increased vulnerability to developing inattentive psychiatric subtypes, such as depression, during adulthood. To better understand this association, in the future, we hope to examine various age groups and consider other socio-demographic variables as potential influencing factors.

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