2015 Student Summer Research Symposium

Bucknell University
Elaine Langone Center
Terrace Room
July 23, 2015
2 p.m. to 4 p.m.

Sponsored by the Bucknell Chapter of Sigma Xi
This symposium has been held for over 20 consecutive years to celebrate the achievements of students doing full-time summer research at Bucknell University. The research is supported with funds from a variety of sources: some students are supported through the \textit{Bucknell Program for Undergraduate Research}, some are supported by the National Science Foundation through \textit{Research Experiences for Undergraduates} grants awarded to departments at Bucknell, and some are supported through faculty individual-investigator grants awarded by organizations like the National Science Foundation and the National Institutes of Health. The Bucknell chapter of Sigma Xi is proud to sponsor this symposium and looks forward each year to seeing the great work being done by students and colleagues. We would like to sincerely thank the students and their faculty mentors for participating in the symposium and supporting student research at Bucknell University. If you would like more information about Sigma Xi, The Scientific Research Society, please contact Dr. Matthew E. McTammany, Bucknell Chapter President, or the national organization’s site (\texttt{www.sigmaxi.org}).

Abstracts are generally organized by departmental affiliation of the faculty mentors, with departments arranged alphabetically, although much of the research highlighted in this session is interdisciplinary. The abstract booklet was compiled by Marty Ligare, Sandy Wendt, and Administrative Services at Bucknell University. Financial support for this session was provided by the Office of the Provost.
Biology

Morphological and Molecular Analysis of *Solanum asymmetriphyllum* × *S. sejunctum* Interspecific Hybrids

Students:  Caton, T A, Jordon-Thaden  
Supervisor: Chris Martine

The overall purpose of this study is to investigate the hybrid offspring produced from the cross of *Solanum asymmetriphyllum* and *S. sejunctum*, two dioecious spiny *Solanum* species from northern Australia. The goal of the study is to determine the morphological and genetic relatedness of the interspecific hybrid offspring, crossed in cultivation for the first time and unknown in the wild, to the parent plants. Both *S. asymmetriphyllum* and *S. sejunctum* have been described morphologically and genetically, which provided evidence that *S. asymmetriphyllum* and *S. sejunctum* are two distinct species. The data collected from this study will either support or refute this speciation event. The methods include morphological measurements of vegetative and floral characteristics, a species-determining restriction enzyme digestion pattern assay using the gene SPOROPOLLENIN, flow cytometry, and Genomic in situ Hybridization (GISH). Once sexually mature, the next step will be to backcross the hybrid plants with both *S. asymmetriphyllum* and *S. sejunctum*, as well as with each other to investigate their reproductive ability. The second generation resulting from the crosses will again be compared, both morphologically and genetically, to the original two study species. Based on collected data, both *S. asymmetriphyllum* male X *S. sejunctum* female and *S. sejunctum* male X *S. asymmetriphyllum* female hybrids more closely resemble *S. asymmetriphyllum*. If future analyses fail to confirm hybridization then it infers one of two things, either that speciation between *S. asymmetriphyllum* and *S. sejunctum* has occurred too recently, or they are not two separate species. Defining a species is important to better guide conservation efforts which may be necessary if the species are distinct because their overall population numbers are reduced, making one or both of the parent species vulnerable. But because our results infer that *S. sejunctum* may just be variable population of *S. asymmetriphyllum*, any conservation efforts may be wasteful. All of these data better explain the evolutionary relationship between *S. asymmetriphyllum* and *S. sejunctum* and provide a better understanding of the mechanisms that isolate these two sister species. Analyzing traits of hybridization as a means of determining evolutionary relationships between species is an unprecedented method that other researchers can emulate in future studies.
**Analysis of Prostaglandin G/H Synthase 2 in bats during white-nose syndrome**

*Student: Brittany Caceres  
Supervisor: Ken A. Field, Ph.D*

White Nose Syndrome is a disease caused by the fungus Pseudogymnoascus destructans (Pd). Pd shows on the bat as a coat of white fungus that spreads around the bat’s muzzle and wing membranes, eating away at them and it is unique because it is a cold loving fungus that grows in the bat’s caves. The disease affects bats in hibernation, causing them to exhibit abnormal behaviors such as flying outside their caves, arousing more frequently, and generally increased activity. It also causes various changes in the bat’s gene expression including, among other things, an increased expression of the inflammatory gene, Prostaglandin G/H synthase 2 (PTGS2). Our research focuses on comparing the responses of the immune systems of the Myotis lucifius (little brown bats) that were affected by White Nose Syndrome with those that were not. The bats were studied during their period of hibernation through their transcriptomes. My role in the project was to use the online, alignment tool, BLAST, to compare the nucleotide and protein sequences of PTGS2 extracted from various bats and to analyze the patterns found through the BLAST searches. It was concluded that only four of the six isoforms were actually useful Prostaglandin G/H Synthase 2 isoforms and the hypothesis that their expression was significantly higher was confirmed.

*Source: This work was supported by the National Science Foundation grant: NSF-DUE-1317446 and the Bucknell University STEM Program for undergraduate students.*

**The Christmas Tree that Keeps on Giving: The invasive potential of cultivated varieties of American Holly**

*Students: Nicolas Diaz, Gabrielle Petruso  
Supervisor: Chris Martine*

The genetic, ecological, and demographic effects of invasive plant species have already been widely documented and studied. The effect of escaped cultivars of native species introduced outside of their natural range, however, has been given little to no attention. This preliminary study sought to locate and identify wild and escaped populations of American Holly (*Ilex opaca*), record sex ratios, and collect sample specimens for future genetic analysis. Site locations were provided by the Pennsylvania Natural Heritage Program. A voucher was collected for each observed population and small tissue samples were collected from individuals within a given population. After the first field season, the study revealed a few noteworthy trends: (1) at locations where Holly was believed to have escaped, high levels of recruitment were observed in shaded understories, (2) a number of populations were observed in riparian zones with noticeably saturated soil, perhaps indicating a selection for a broadened soil tolerance, and (3) Holly
thrive in disturbed forests and edge habitats where other common invasive species occurred. Determining whether an individual was sexually mature proved difficult when drupes were not present. However, a slight male bias in some populations was observed. Upcoming comparisons of populations using genetic tools will determine future directions of the study.

**Sources of support:** David Burpee Endowment, Wayne E. Manning Internship Fund, Botanical Society of America Undergraduate Research Award, NSF STEM Scholars Program

**Celebrating difference:** Morphological comparison between a narrowly-endemic Australian species (*Solanum eburneum*) and a locally-recognized variant.

**Student:** Emma Frawley  
**Supervisor:** Chris Martine, Ingrid Jordon-Thaden, Rachel Martine

The monsoon tropics of northern Australia are home to many endemic species, including numerous spiny solanums (*Solanum subgenus Leptostemonum*). *Solanum eburneum* is an andromonoecious species restricted to clayey soils in the vicinity of the East Baines River, Northern Territory, with a range largely encompassed within Judbarra/Gregory National Park. For at least 30 years, regional botanists have recognized a subpopulation of *S. eburneum* as *S. ‘bullita’* but no formal comparison between it and typical *S. eburneum* has been done. The current study represents the first rigorous morphological comparison between the two taxa using data garnered from seedlings through mature plants, including measurements of vegetative, floral, and fruiting characteristics. Using plants grown from wild-collected seeds, morphological analyses are combined with molecular phylogenetic comparisons, crossing experiments, and field observations to establish the distinctive nature of *S. ‘bullita’*. The implications of recognizing the new taxon are explored, including potential effects on the conservation status of *S. eburneum*.

**Support:** Bucknell University, David Burpee Endowment, BSA Undergraduate Research Award, Wayne E. Manning Internship Fund
Resource allocation and flower plasticity Australian nightshade *Solanum clarkiae*.

**Student:** Fonseca, F.V.B  
**Supervisor:** Martine, C.T

The focus of this study was to analyze the floral plasticity and the responses of resource allocation on the Australian nightshade *Solanum clarkiae*. Four treatments were produced for this experiment: “No Males”, where the males’ flowers were removed while early buds, “No Hermaphrodite”, where the hermaphrodites were removed while early buds, “No Fruit”, where hermaphrodites were removed after flowering and “Plus Fruit”, where hermaphrodites were hand pollinated in order to produce fruits. Twelve measurements were taken from the flowers but previous work found that corolla diameter may be the best indicator, among these measurements, for visualizing responses to resource allocation (Vasconcelos and Proença, 2015). For the “No Males” treatments, significant difference for corolla diameter was seen when a comparison was made between hermaphrodites from control and samples. The opposite was found for “No Hermaphrodites” treatment, where no difference in the corolla diameter was found. Two plants for the “No-Fruit” treatment presented hermaphrodites on the distal part of the inflorescence and no difference was found on the comparison of the corolla diameter for the male flowers. Only four plants of the “Plus-Fruit” treatment set fruit and for those, no difference on the corolla diameter and the number of males flowers was found. Based on the results, we found evidence for floral plasticity in *Solanum clarkiae*. For three of the treatments, significant variation was seen when compared to controls. Future studies involving quantification of pollen will be needed in order to better understand the resource allocation for the “No Hermaphrodite” treatment. Overall, a larger sample size may be the best option to fully understand the pattern of plasticity in this species.

The source of support for this work was provided by Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), number of the procedure: 88888.072256/2013-00 and the David Burpee Endowment at Bucknell.

**Effects of Short Term Stress on Glucocorticoids and Antioxidants**

**Student:** Dasha Kostyuchek*  
**Supervisor:** Elyse K. McMahon, Hannah P. Litwa, Mark F. Haussmann

Reactive oxygen species are a normal consequence of energy metabolism and are implicated in the aging process. Antioxidants are one defense mechanism against oxidative damage produced by reactive oxygen species. High levels of glucocorticoids experienced during chronic stress are associated with decreased levels of antioxidants. While less is known about how acute stress affects antioxidants, recent research suggests that even over short periods, antioxidant levels decrease. We conducted an acute stress
test on Japanese quail (*Coturnix japonica*) to determine the effects of corticosterone on antioxidant levels. Blood samples were collected before (baseline sample), 20 minutes into (stress-induced sample), and 45 minutes after initiation of a mild restraint stress (recovery sample). In these samples, we measured corticosterone, the main avian glucocorticoid, and total antioxidant capacity. We report that compared to baseline and recovery corticosterone levels, stress induced corticosterone levels were higher. In addition, over the course of an acute stress response, there was a decline in total antioxidant capacity. While chronically elevated glucocorticoids can lead to decreased antioxidant defenses and age related disease, our results suggest that even transient stress may have negative consequences.

Support: Bucknell University STEM Support to DK and a National Science Foundation Award to MFH

**Effect of fire on seed germination in *Solanum beaugleholei*, an endemic spiny solanum of the Kimberley region, Australia.**

**Student:** Laryssa Gavala  
**Supervisor:** Christopher Martine, Ingrid Jordon-Thaden, Rachel Martine

Spiny solanums of the fire-prone Australian monsoon tropics are often assumed to be “fire weeds,” with increased levels of recruitment associated with frequent bush fires. During fieldwork on the Kimberley Plateau, seeds of the endemic *Solanum beaugleholei* were collected from a habitat where an intense fire had recently burned. Seeds were removed from fruits exposed to three qualitative levels of burning: scorched, partially burned, and unburned. Fruits/seeds were then collected from an unburned *S. beaugleholei* population ca. 25 km away. In the lab, half of the seeds of each of the four “fire treatments” were soaked and treated with gibberellic acid, while the other half were soaked in water only. To understand the effect of the fire on the seeds, time to germination and rates of germination were recorded. Seeds collected from the unburned population and unburned seeds from the fire site showed the highest germination rates and shortest time to germination, allowing us to infer that fire has a negative effect on seed germination in *S. beaugleholei*. As a means to further confirm and clarify these findings, the seedlings were grown into mature greenhouse plants and hand pollinated to establish a new seed source for experiments replicating fire conditions ex situ. Seeds were given pre-sowing treatments exploring the potential roles of various ecological correlates of fire exposure in hastening or promoting seed germination and seedling growth. Understanding the effect of fire on *S. beaugleholei* may be useful in conservation efforts. Because fire appears to hinder seedling recruitment in *S. beaugleholei*, frequent incidences of fire (including prescribed burns) on the Kimberley Plateau could result in declines of this uncommon endemic species in certain habitats.

Funded by: Botanical Society of America Undergraduate Research Award, David Burpee Endowment, NSF STEM Scholars Program.
Exploring the potential for *Solanum* fruit ingestion and seed dispersal by rock-dwelling mammals in the Australian monsoon tropics.

**Student:** L. Mae Lacey  
**Supervisors:** Elizabeth Capaldi, Ingrid E. Jordon-Thaden, Christopher Martine

Little is known about the methods of seed dispersal employed by rock-specialist spiny solanums (*Solanum* subgenus *Leptostemonum*) in the monsoon tropics of northern Australia. Previous studies infer that endozoochory may play a role, but no specific animal taxa have been identified as effective seed dispersers. The elusive rock macropod species co-occurring with solanums are potential candidates, particularly species of *Petrogale* (rock wallabies) and *Macropus* (wallaroos). To assess the potential of these animals as seed dispersers, a study is underway to determine whether rock macropods might ingest *Solanum* fruits and pass seeds intact. Eight *Solanum* taxa endemic to northern Australia were grown from wild-collected seeds hand-pollinated at flowering maturity, and then used as sources of fruit. Ripened fruits will be presented to rock macropods in captivity to determine the following: a) Will rock macropods consume *Solanum* fruits, and which species?, and b) Do the seeds consumed with the fruits survive gut passage? Intact seeds were removed from scats and sown to test for germinability compared with uningested seeds. Determining whether co-occurring species of mammals participate in successful endozoochorous *Solanum* seed dispersal has implications for conservation efforts by highlighting the importance of plant-animal interactions among narrowly endemic species. Here we present preliminary data, including experiments on seed gut passage time and germination rates following ingestion by captive rodents as proxy subjects.

Sources of support: David Burpee Endowment, Wayne E. Manning Internship Fund, Botanical Society of America Undergraduate Research Award

**Preparation of spider spermatocytes for Electron Microscopy by embedding cells in a clot**

**Students:** Makayla Lagerman and Sabrina Malagón  
**Supervisor:** Dr. Le Paliulis

Spiders have the widest variety of chromosomal sex determination mechanisms of any order. The sex chromosomes, because they are present in different numbers and arrangements than autosomes, display interesting behaviors during spermatocyte cell division. To understand these interesting chromosome movements, analysis by electron microscopy (EM) is required. Sample preparation of spermatocytes for EM is typically very difficult and unreliable because spermatocytes do not adhere to a substrate. To immobilize cells, we embedded them in a clot them using a mixture of fibrinogen and thrombin. The samples were fixed and left overnight in fixative mixed with buffer. Both
a PIPES and a phosphate buffer were tested as a vehicle for fixation. We found that using the phosphate buffer led to better preservation. Samples were then prepared for electron microscopy using standard methods. By embedding spermatocytes in a clot and fixing using a phosphate buffer, we were easily able to obtain quality samples for EM and future sectioning.

**Identification and Isolation of Novel Arthrobacter Phage**

**Students: Hayalneh Gessesew, Lara Nunn**  
**Supervisor: Marie Pizzorno**

Bacteriophage (also known as phage) are viruses that infect and replicate within bacteria. The host bacterial species we worked with was Arthrobacter which can be found in soil. Previous work had difficulty identifying novel phage that can infect Arthrobacter. Our goal was to improve phage hunting in this bacterial species. After obtaining soil samples from two different sites across campus, we attempted to isolate any existing Arthrobacter phage in the soil using a modified enrichment protocol. By altering the method of phage isolation, the goal of the project was to determine the ideal conditions to isolate phage that infect Arthrobacter. We found that this modified protocol yielded several different kinds of plaques. A second goal of this project was to identify which phage belong to the AN cluster as early in the isolation process as possible. PCR was carried out using primers designed to flank the variable region of the AN cluster Arthrobacter phage genomes. PCR was carried out on isolated DNA, phage lysate, and isolated plaques. The results of these experiments will be discussed.

Funding source: NSF STEM Scholars Grant, Department of Biology
Biomedical Engineering

Comparison of Magnetic Resonance Imaging Techniques in Assessing Left Ventricular Strain

Student: Jared Feindt
Supervisor: Christopher Haggerty

Functional parameters of left ventricular (LV) contraction are an important marker of heart disease. For example, LV strain—a measure of how much the heart wall deforms while pumping blood—has been reported in many studies and shown to be a good predictor of poor outcomes. Several options for calculating strain exist, with commercial “feature tracking” (FT) software being the most common. Displacement encoded (DENSE) imaging is a more robust method that directly measures cardiac motion and may provide more accurate results. The goal of this study is to compare these two magnetic resonance imaging (MRI)-based approaches for quantifying the mechanics of LV deformation. We hypothesize that measurements of LV strain from FT analysis and DENSE will have good agreement. Cardiac MRI data were acquired in 25 healthy volunteers (23.2±17.1 years) and 18 patients with heart disease (17.0±23.8 years). Each subject had two imaging sequences performed: 1) standard anatomical imaging, and 2) DENSE imaging. For this study, we selected all instances in which these acquisitions were performed at the same spatial location to facilitate direct result comparison. Across patients, 93 imaging planes (68 ‘short-axis’, 25 ‘long-axis’) met this criterion. Commercial FT software was used to semi-automatically track heart motion in the anatomical images to compute strains. DENSE images were post-processed using custom MATLAB software. Short and long-axis images were used to compute circumferential and longitudinal strains, respectively. Agreement was assessed using Bland-Altman limits of agreement and the coefficient of variation (CoV). The average circumferential strain in FT and DENSE was 26.5±9.2% and 17.3±3.8%, respectively. The average longitudinal strain in FT and DENSE was 27.9±6.9% and 13.4±2.2%, collectively resulting in a mean bias of 10.2%. Furthermore, the limits of agreement were large with respect to the measurement means (CoV = 36%), indicating poor agreement. These results strongly suggest that the limitations of FT software’s ability to track features cause systematic measurement bias. Such bias indicates that DENSE is more clinically appropriate for patients where small changes in strain are relevant. Future work will examine the effects of 3D cardiac motion on LV strains measured through DENSE acquisition and analysis.

Support: Weis Center for Research
Chemical Engineering

Quantifying Hydrogel Degradation using a Millifluidic Device: A Model for In Vivo Drug Delivery

Student: Ounyae Williams; Co-Worker: Madeline Milligan
Supervisor: Erin Jablonski

The delivery of drugs into the human body is typically accomplished through oral delivery (capsules, tablets, etc.) or parenteral delivery (injection). For drugs that must be taken at regular intervals over long periods of time, issues such as patient compliance (forgetting to take medication, aversion to needles) and periodic dosing (resulting in high, side-effect causing toxic concentration in the blood metabolized to a low, ineffective concentration) result in waste of drug and little time spent in the therapeutic range of drug concentration in the blood.

In this work the overall purpose is to evaluate a degradable hydrogel material that may be suitable for controlled drug delivery. The hydrogel of interest is dextran-methacrylate (dex-MA), and the system of interest is a microfluidic device in which laminar flow at low volumetric flow rates allows a comparison to conditions in vivo. Thus far in the project we have successfully fabricated dextran-methacrylate loaded microfluidic devices and tested these devices with model aqueous solutions. Devices are prepared by creating a glass-on-glass shell sealed with an elastomeric adhesive membrane, and subsequently photo-curing an aqueous solution of dextran-methacrylate and a photo-initiator, using a photomask and needle to define the microfluidic channel. The current fabrication technique is a significant improvement over former methods due to the ability to rapidly prototype devices with inexpensive materials. To monitor the interaction of the flowing aqueous solution with the degradable hydrogel, images are captured at regular intervals. With these images, the width of the channel is quantified over time and the rate of degradation is calculated.

During our initial studies we have attempted to test various solutions to observe which solution will cause the hydrogel to degrade and/or dissolve faster. These experiments are in progress; however, based on based on preliminary results and prior work (Ellenberger Thesis, 2013), we have developed three hypotheses: 1. dex-MA should degrade/dissolve at a greater rate when contacted with a solute-free aqueous stream as compared to an aqueous buffer solution due to the increased solubility of the dex-MA degradation products in the solute free aqueous stream; 2. dex-MA should degrade/dissolve at a greater rate when contacted with an acidic solution as compared to a neutral solution due to the pH of dex-MA degradation products; 3. the dex-MA rate of degradation/dissolution should be directly related to the volumetric flow rate in the microfluidic channel due to lower local concentration of degradation products. To test these hypotheses, the following experiments are planned using a formulation (30 wt. % dex-MA with 70 wt % de-ionized water with photo-initiator) that has been photo-cured in microfluidic devices.
with brilliant black aqueous solution as the model to allow for image contrast between the hydrogel and microfluidic channel.

Grant: NSFDUE-1317

**Morphology of Even Dicarboxylic Acids**

**Student:** Katherine F. Warfel  
**Supervisor:** Dr. Ryan C. Snyder

Organic molecular particles play an important role in many different applications including foods, specialty chemicals, and pharmaceuticals. Three characteristics that strongly influence performance of organic molecular particles are size, morphology (shape) and internal structure (arrangement of the molecules in the solid state). The morphology refers to the surface properties and the specific shape that a particle exhibits and affects particle functionality and its ability to be processed. Using different methods to produce particles can result in unique morphologies. In this work, particles with uniform size and shape are produced from solutions using monodisperse droplet evaporation technology. Monodisperse droplet evaporation is achieved using a Vibrating Orifice Aerosol Generator (VOAG). The VOAG produces monodisperse droplets from a solution, which then rapidly evaporate in a collection column, leaving particles to be examined. In these morphology experiments, the solution includes a pure organic dicarboxylic acid as a solute in an organic solvent. The solute acts as a model active pharmaceutical ingredient. Many factors affect the morphology of a particle, but this experiment focuses on the choice of solute and solvent. In this work, the surface morphology and internal structure are examined for several even dicarboxylic acids such as Suberic Acid (C8) and Sebacic Acid (C10). Solvents tested include Isopropanol, Acetone, Methanol and Ethanol. A Scanning Electron Microscope (SEM) is used to examine shape and surface morphology as well as internal structure and morphology once particles are cracked open. The crystalline nature of the particles is confirmed using an X-Ray Diffractometer (XRD). Results are compared within these experiments and to existing characterizations. Applications for specific morphologies are also considered.

Source of Support: Bucknell Program for Undergraduate Research
Chemistry

Aerosol Formation Rates in the Presence of Different Bases: Ammonia, Methylamine and Mixed Ammonia-Methylamine

Student: Nana Appiah-Padi*
Supervisors: Berhane Temelso, George C. Shields
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Aerosol particles in the atmosphere reflect back sunlight and regulate the lifecycle of clouds. Our work focused on ternary sulfate aerosols containing methylamine (MA, CH₃NH₂), ammonia (A, NH₃), the combination of the two (MA-A) and sulfuric acid dimers (S₂) and compared their effectiveness in new particle formation in the atmosphere. We chose S₂–MA₂, S₂–A₂, and S₂–MA–A because recent experiments have shown that the presence of heterogeneous bases (MA–A) enhances aerosol formation significantly more than homogeneous bases (A and MA) alone. This work attempts to explain this phenomenon using computational tools. To sample the possible configurations, we used genetic algorithm with semiempirical methods. For each system, the unique low energy structures from the final pool of 500 clusters were minimized using a density functional method. These structures were finally run through more rigorous density functional methods with a larger basis sets. Although experimental measurements showed that there was a greater new particle formation rate for the MA–A system, followed by MA₂ and A₂, the computed binding energy of the clusters follows a different order: MA₂ > MA–A > A₂. The reasons for these differences between computation and experiment are explored.

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Probing Chiral Recognition in Bile Salt Micelles Using Isothermal Titration Calorimetry

Student: Shauna L. Anderson
Supervisor: Timothy G. Strein, David Rovynak

It is well known that bile salts form micelles that are capable of stereo-specific binding of binapthyl guest molecules, but the precise structure, energetics and dynamic behavior of these micelle systems remains elusive. In this work, isothermal titration calorimetry (ITC) is used to characterize the thermodynamics of the sodium cholate bile salt micelle system, providing information about the stability and stoichiometry of chiral interactions.
between cholate micelles and model binapthyl compounds. ITC is shown to be well suited for measuring the difference in micelle-binding energetics between the R- and S-enantiomers of 1,1’-bi-2-naphthol (BN) and 1,1-binaphthyl-2,2’-diylhydrogenphosphate (BNDHP), molecules that are known to bind to cholate micelles with differing affinity. Binding is clearly entropically controlled, but chiral selectivity is mapped by the enthalpic contribution. These experiments have provided a direct measurement of thermodynamics of stereo-selective guest solubilization of binapthyl substrates by bile micelles. In addition to thermodynamic data, our demicellization experiments yield cmc values for the cholate system under various conditions, and quantify the energy difference (< 1 kJ/mole) for the binding energies between the two enantiomers of BNDHP. Moreover, high concentrations (above 0.6 mM) of BNDHP are shown to mediate the cholate micellization process. In all, ITC data that systematically investigate the cholate micelle system, as well as the binding of BN and BNDHP to cholate micelles, will be presented.

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**Comparing Single and Multiple Base Systems in Secondary Aerosol Formation**

**Student: Fern Morrison**
**Supervisors: Berhane Temelso, George C. Shields**

Atmospheric aerosols have a great impact on our global climate. They cool the planet directly by reflecting light away from the earth, and indirectly by acting as cloud condensation nuclei that regulate the lifespan of clouds. Despite their importance in the earth’s radiation balance, the lack of understanding about their formation has led to uncertainties about their effect on the global climate. Of all the common aerosol particles, sulfate have the most significant cooling effect and their formation is enhanced by the presence of bases like ammonia amines. Recent experiments have shown a synergetic effect between ammonia and amines which yields aerosol formation rates substantially larger than from each of the bases alone. This study attempts to explain that synergistic behavior by exploring the clustering of sulfuric acid H2(SO)4, ammonia NH3, and trimethylamine (CH3)3N. Initial configurational sampling was performed using genetic algorithm to find a large number of low energy configurations. These structures were then subject to quantum mechanical calculations. The thermodynamics of formation for the most stable structures was then calculated. The combined data showed that the binding energy of the cluster is related to the base dissociation constant (pKb) value of the base. Calculations also showed that S2-TMA-TMA had a lower binding Gibbs free energy (ΔG) than S2-TMA-A and S2-A-A. This disagrees with experimental observations and the reasons for this discrepancy are explored.
Funding sources: NSF STEM Talent Expansion Program (STEP) grant DUE-1317446 and NSF RUI grant CHE-1213521.
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Atomic Force Microscopy Investigation of Heterogeneity in Smectite Swelling

Students: Diana S. Arndt, William A. Peterson
Supervisor: Dr. Molly M. McGuire

Understanding the swelling capabilities of clay minerals has the potential to benefit fields such as civil engineering, pollution control and the drilling industry. Smectites, clay particles with the ability to swell, have a layered crystalline structure with silicate sheets encompassing layers of cations. The space between these layers is not fixed; water can be absorbed into the quasi-crystal structure, resulting in swelling. Atomic force microscopy (AFM) is used to image these clay quasi-crystals in situ as they swell. The corresponding software produces topographical images of the particles at different times throughout the swelling process. These images can be compared and interpreted to determine swelling behavior and rate. Previously, questions about the swelling rate of quasi-crystals were difficult to explore because there was no process established to analyze the swelling behavior across the entire particle. However, this study has organized a method of creating a z, or height, value threshold on an AFM image to isolate a plane of the quasi-crystal, which can be compared to subsequent images of the same particle plane later in the swelling process. The difference in area of these two planes is interpreted as evidence that swelling or deswelling has occurred, and to what extent. The analysis of AFM images in this study has shown heterogeneous swelling patterns based on what layer of the particle is examined. Presumably, this heterogeneity can be explained by variable layer charge resulting from random isomorphic substitution of cations within the quasi-crystal structure of the clay mineral.

Effects of Mutation at Position 557 on the Catalytic Properties of Soybean Lipoxygenase-1

Student: Natasha F. Bassett
Supervisor: Charles H. Clapp

Soybean lipoxygenase-1 (SBLO-1) is a non-heme iron protein that catalyzes the oxygenation of polyunsaturated fatty acids to hydroperoxides. With linoleic acid as substrate, oxygenation occurs almost entirely at carbon-13, with some oxygenation at carbon-9. Though the three-dimensional structure of the enzyme is known, it is not certain how substrates bind. Since SBLO-1 has a binding pocket with an iron along the
side, and a phenylalanine residue at amino acid position 557 (the interior of the pocket), it is hypothesized that substrates bind tail-first to this active site, with the terminal methyl group of most substrates interacting with the phenylalanine ring. Under this hypothesis, by changing the residue at position 557 to a smaller residue, oxygenation should occur more at position 9, as the substrate has more room to “back in” to the binding pocket.

Site-directed mutagenesis was completed on the enzyme at position 557 to change the phenylalanine to a valine (mutant F557V) and serine (mutant F557S) residue. The serine mutant was found to have a much lower activity than the wild type enzyme, and experienced substrate inhibition. The valine mutant showed increased amounts of oxygenation at the 9 position of linoleic acid, the substrate, which we proposed to be due to tail-first binding.

Current work on the F557V mutant involves linoleoyl-D-valine and linoleoyl L-valine, two stereoisomers of the same substrate. If our working hypothesis of reverse binding holds true, the amount of 9-oxygenation seen in the products should depend on the stereochemistry of the substrate.

Department of Chemistry, Bucknell University
NSF RUI CHE-1213262

Low temperature controlled radical polymerizations of vinyl aromatic monomers

Student: Christine Bendzinski
Supervisor: Dr. Eric Tillman

It is well-known that it is not only the monomer identity that affects the properties of polymers, but also the stereochemical configuration of the pendant groups along the chain. A series of possible methods for low temperature radical polymerizations of vinyl styrenic monomers was explored, with the ultimate goal being control over the stereochemistry of the polymers by maximizing intermolecular interactions. The interaction of interest to this work, called pi-pi stacking, is known to occur between electron rich and electron deficient aromatic systems. Pentafluorostyrene and styrene were used as monomers to make alternating copolymers, and the progress of these reactions was monitored by NMR and GPC analyses. The guiding hypothesis is that these pi-pi stacking interactions may impart stereoregularity in the polymer as a consequence of the strong intermolecular interactions and thus orientation of the monomers prior to being incorporated into the polymer chain. This work has shown that low temperature radical polymerizations, down to ambient temperatures, are possible, while NMR has shown the interaction of the aromatic and vinyl groups of the monomers.
Characteristics of the Colloidal Phase of Acid Mine Drainage from Shamokin, Pa

Students: Joyce Obeng, Sarah Bradley  
Supervisor: Molly McGuire

Colloids, the smallest suspended particles in natural waters, have the unique ability to transport adsorbed organic material and metals downstream. Aggregation of colloids can result in the eventual destabilization of the particles which will fall to the stream bed, potentially increasing the metal or contaminate concentration in the sediment. To better understand the potential for contaminate transport, the characteristics of the colloid must be determined in the laboratory. When studying a natural acid mine drainage (AMD) sample in the lab, care must be given to degradation occurring as the sample is removed from its environment. In this study, samples underwent varying laboratory conditions to determine the lifespan of samples in the laboratory. Samples were ultra-filtered to concentrate the colloidal particles. The aqueous sample was analyzed using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR). Temperature, age, and pH of samples were investigated. Evidence of the minerals schwertmannite and goethite were identified in both the warm and cold samples, with increasingly clear peaks as the sample aged. Changes in pH resulted in significant changes in mineralogy of colloids, indicated both by characteristic color changes and the spectra.

Source of Funding: NSF-DUE-1317446, 2015 Summer Research Fellowship from the Office of Graduate Studies

Hydration of Sulfuric Acid-Methylamine Clusters in the Atmosphere

Student: Bobby Cao  
Supervisors: Berhane Temelso and George Shields

Sulfuric acid (H_2SO_4) is the main driver of aerosol formation and the presence of bases like ammonia and methylamine (CH_3NH_2) stabilize molecular clusters and enhance aerosol formation through a process called ternary nucleation. We are studying the formation of particles that include sulfuric acid dimer (H_2SO_4)_2, methylamine and up to three water (H_2O) molecules. Thousands of clusters of the form (H_2SO_4)_2(CH_3NH_2)(H_2O)_n, n=0-3, were initially generated by using genetic algorithm. Then the most stable clusters were studied more rigorously with quantum mechanical methods. The addition of methylamine stabilizes the sulfuric acids substantially, but it does not affect the subsequent hydration thermodynamics significantly. Acid dissociation of one or both sulfuric acids is accelerated in the presence of methylamine compared to binary (H_2SO_4-H_2O) systems.
Alternative sampling densities compared to exponential weighting in non-uniform sampling

Students: D. Levi Craft, Melissa R. Palmer, Philip Stahlfeld, Supervisor: David Rovnyak

Non-uniform sampling (NUS) is more widely practiced, but many implementations either do not weight the distribution of samples, or follow exponential sampling densities. Weighting the sampling density in proportion to the signal envelope provides intrinsic sensitivity enhancements (MRC, V49, 483-491, 2011). However sinusoidal weighting is a compelling alternative to exponential weighting matched to the signal decay (JBNMR, V58: 303-314, 2014). We now describe families of alternative densities as candidates to replace common exponential NUS weightings. Yielding equal intrinsic sensitivity to their exponential counterparts, these alternatives possess improved constraints on line shapes by distributing more samples beyond 1xT2. An algorithm to generate properly gapped sampling densities (JBNMR, V58: 303-314, 2014) is extended, and is also contrasted with deterministic NUS schedules.

Support: Drs. Anthony and Joyce D. Kales Fund

Chemical Synthesis of Bile Acid Analogs for Immunological Evaluation

Students: Jack E. Geduldig, Ryan K. Eng
Supervisor: Michael R. Krout
Co-authors: Katie M. Lewis, Jun R. Huh

Recent studies have shown the potential for the secondary bile acid lithocholic acid (LCA) and its C(5) diastereomer allolithocholic acid (alloLCA) to modulate regulatory T-cells (T_{reg}) found in the gastrointestinal tract. These immune cells are important in the regulation of intestinal inflammation and serve a critical role in the maintenance of immune homeostasis. Our efforts to devise a chemical synthesis of alloLCA have facilitated access to a number of synthetic intermediates that we have used to prepare a variety of analogs with novel chemical structures. The current study focused on the chemical modification of the A-ring of the steroid nucleus as well as the C(17) alkyl side chain. We aim to use chemical synthesis to improve our understanding of the
relationship between structural features and cellular activity in order to design improved analogs.

Supported by the Harold W. Heine Undergraduate Research Fund in Chemistry and the Drs. Anthony and Joyce D. Kales Undergraduate Research Fund

Application of Functionalized Organozinc Reagents for the Synthesis of Complex Sesquiterpenes

Student: Tyler J. Fulton
Supervisor: Dr. Michael Krout

The addition of functionalized organozinc reagents to α,β-unsaturated carbonyls has been investigated with emphasis on forging quaternary stereocenters in an effort to develop an efficient and selective double-addition strategy towards the synthesis of sesquiterpene natural products. Initial screening of a substrate scope of this semi-optimized chemistry and application to total synthesis of β-eudesmol are presented.

Support for this Work American Chemical Society Division of Organic Chemistry SURF program

Generation of Metallopolymers Using Transesterification

Students: Kevin Garcia, Kurt R. Vostal, Wade E. Heidel
Supervisor: Robert Stockland

Abstract: Metallopolymers have been generated through transesterification reactions using both conventional and microwave heating. A variety of monomers bearing a number of different functional groups were incorporated into the polymer chain in order to change the physical properties of the polymer. The presentation will outline the effectiveness of this approach to the preparation of metallopolymers with prescribed physical properties.

Source of support for the work: National Science Foundation
Nature uses metal ions associated with proteins (metallocofactors) for a range of purposes, often exploiting the Lewis acidity or redox activity of the metal ion to accomplish a particular chemical transformation. In some cases, cofactors consist of different metals in close proximity that work cooperatively together. The recently discovered class Ic ribonucleotide reductase (RNR) R2 subunit is one such protein, utilizing a Fe/Mn cofactor to transfer electrons during DNA synthesis. In this work, we investigate how the cofactor is selectively assembled given the similarities of Fe and Mn, which are neighboring elements on the periodic table. Initially the symmetrical ligand, 5-R-2-hydroxy-1,3-xylene-α,α′-diamine-N,N,N′,N′-tetraacetic acid (abbreviated R-HXTA, R = CH₃, F), was used to study the preference for the three possible cofactors (Fe/Fe, Mn/Mn, and Fe/Mn). This was done by measuring the amounts of each species present using nuclear magnetic resonance (NMR) spectroscopy. Next, our goal became synthesizing a nonsymmetrical HXTA ligand with one “high affinity” site and one “low affinity” site. Our motivation was to better mimic RNR, which has two different metal binding sites. The symmetrical ligand contains two chelating rings of the same size (5-membered), whereas the nonsymmetrical ligand has one 6-membered chelate ring to decrease metal binding affinity. The R substituent was also moved from the para to the meta position aid characterization of the complexes by NMR. The future work will compare the preference of each cofactor in the symmetric model versus the nonsymmetric model and determine the equilibrium constants for the different complexes.

This work was supported by the American Chemical Society Petroleum Research Fund (50877-UNI3).

Radical Trap-Assisted Atom Transfer Radical Coupling of Diblock Copolymers to Form Triblock Copolymers

Students: Julie Herman, Jess Abruzzese
Supervisor: Dr. Eric Tillman

Synthesis of a polymer chain with a functional end group can be achieved through Atom Transfer Radical Polymerization (ATRP). These polymer chains can then be utilized in further reactions through the functional end group. Sequential ATRP reactions can be used to form diblock copolymers by utilizing the end group functionality of the first and using it as the macroinitiator for the second ATRP reaction. These end brominated diblock copolymers can then be subjected to radical trap assisted-atom transfer radical
coupling reactions (RTA-ATRC), resulting in ABA type triblock copolymers. The use of sequential ATRP reactions followed by RTA-ATRC was shown to be a successful method to form triblock copolymers using different monomer combinations. The RTA-ATRC was successful when done using diblock copolymers containing either styrenic or acrylic end groups, resulting in triblock copolymers in high yields that could be isolated by fractionation. The polymeric products were analyzed using size exclusion chromatography and nuclear magnetic resonance (NMR).

Funding Source: National Science Foundation

Utilization of 9,12 eicosadienoic acid as a novel substrate to test the tail-first binding theory of soybean lipoxygenase-1

Student: David Hinnenkamp
Supervisor: Dr. Charles Clapp

Soybean Lipoxygenase-1 (SBLO-1) is a nonheme-iron enzyme that catalyzes the conversion of linoleic acid into predominantly 13-hydroperoxyoctadecadienoic acid (13-HPOD), and less frequently, 9-hydroperoxyoctadecadienoic acid (9-HPOD). Although the amino acid sequence and the three dimensional structure of SBLO-1 are known, uncertainty still exists as to how the linoleic acid substrate binds in the SBLO-1 active site. Previous studies suggest the theory of tail-first binding, where the hydrophobic carbon-hydrogen chain of linoleic acid enters first into the binding site and establishes stable interactions with the phenylalanine ring (557). To test this theory, a substrate with two additional carbons on its tail end, 9,12 eicosadienoic acid (9,12 EDA), was synthesized. Multiple assay experiments were performed using WT SBLO-1 and F557A mutant enzyme with both linoleic acid and 9,12 EDA. Early results suggest linoleic acid is a better substrate than 9,12 EDA with the WT SBLO-1 at both low (1µM) and high (50µM) substrate concentrations, as shown by its higher activity level. However, the activity levels of linoleic acid and 9,12 EDA were considered identical within error at low (1µM) substrate concentrations with the F557A mutant. Linoleic acid and 9,12 EDA had values, respectively, of .33 ± .05 µM/min and .35 ± .10 µM/min when assayed with the F557A mutant. The results from the aforementioned assay experiments, with both WT SBLO-1 and the mutant F557A enzyme, support the tail-first binding theory. Product determination experiments using 9,12 EDA as a substrate with WT SBLO-1 and F557A mutant are currently in progress.

Support: NSF-RUI CHE-1213262
Development of a Stereoselective Synthesis of Allolithocholic Acid

Student: Samantha P. Kelly, Brandon N. Nelson
Supervisor: Michael R. Krout
Co-author: Jun R. Huh

Recent studies have found that bile acids, in addition to serving for regulation and absorption of lipids and other fat-soluble compounds in the gastrointestinal tract, can also function as cell signaling molecules. Specifically, allolithocholic acid (alloLCA), a structural derivative of the naturally occurring bile acid lithocholic acid (LCA), has shown potential to activate regulatory T cells found in the GI tract. Due to the high cost and limited access to commercially available alloLCA and derivatives thereof, we have explored methods of chemical synthesis to produce alloLCA from the inexpensive, commercial LCA. Because alloLCA is epimeric at C(5) relative to LCA, this conversion is not trivial. After a two-step oxidation process to convert LCA into an α,β-unsaturated ketone, our efforts have focused on the stereoselective reduction of the substrate using various methods.

Supported by the Bucknell Program for Undergraduate Research and the Office of Graduate Studies.

New Cross-Coupling Method for Flame Retardant Material

Student: Taylor M. Lord
Supervisors: Kevin J. Garcia, Stephanie L. Casino, and Robert A. Stockland Jr.

A new method is being tested in the development of flame retardant material. Currently, there are very few safe methods for the synthesis of flame retardants, and this method has proven to be successful due to the halogen-free products. A range of compounds have been synthesized and investigated as catalysts for a cross-coupling reaction in order to find the most efficient catalysts. Cross-coupling pentaerythritol with a compound with different substituents has proven to be successful.

Source of Support for the work: PRF
Explaining the Increased Sulfate Aerosol Formation Rates in Mixed Ammonia-Dimethylamine Systems

Student: Grace Kim
Supervisor: Berhane Temelso, George C. Shields

Composed of gas phase molecules found in the atmosphere, aerosols form through a nucleation process before serving as cloud condensation nuclei (CCNs) that seed clouds. Aerosols have been found to have a net cooling effect on the global climate, but the process of their formation is still not well-understood. Acid-base reactions between sulfuric acid [H₂SO₄, S] and ammonia [NH₃, A] promote aerosol formation and the effect is even greater for amines. Recent studies have shown the presence of ammonia and amines increases aerosol formation rates significantly more than ammonia or an amine alone. For this study, dimethylamine [(CH₃)₂NH, DMA] was chosen due to its stronger basicity and larger size. The possible configurations of S₂-DMA-A and S₂-DMA₂ were sampled using a genetic algorithm applied on semi-empirical potential energy surfaces. The low energy structures were subject to quantum mechanical calculations with large basis sets. From our data, we have come to the conclusion that binding energies strongly correlate with the basicity of the base: S₂-DMA₂ > S₂-DMA-A > S₂-A₂. These conclusions disagree with experimental nucleation rates which increase in the order S₂-DMA-A > S₂-DMA-DMA > S₂-A₂. The reason for these discrepancies are explored.

Funding sources: The Bucknell Undergraduate STEM Research Program and NSF STEM Talent Expansion Program (STEP) grant (DUE-1317446) and NSF RUI grant (CHE-1213521)
Computing resources: MERCURY Consortium (NSF MRI grant CHE-1229354) and Texas Advanced Computing Center (TG- CHE090095 and TG- CHE120025)

Improving an In-Capillary Assay for Creatinine: Stacking the Jaffe Product

Students: Abigail F. Kreznor, Elizabeth J. Seidell
Supervisor: Timothy G. Strein

Capillary electrophoresis (CE) is a low volume, high efficiency technique that is based upon differential migration rates of ionic species. In this research, a few nanoliters of a sample solution containing creatinine, a neutral clinical marker for renal failure, is injected into a CE capillary and mixed with picrate which has anionic mobility. The Jaffe product which is formed proportionally to the creatinine content in the sample, is bright red, and can be easily separated from the mixture. The goal of this project is to optimize the conditions to achieve ideal peak height and width of the Jaffe product. Some conditions that effect the Jaffe reaction are reactant concentrations, injection lengths, overlap times, and buffer conditions. To enhance the method a technique known as stacking has been applied to the in-capillary Jaffe reaction. During the stacking process,
analytes at low concentrations in a long sample zone are focused into a short, more concentrated zone (stacked). Hydroxide is used to promote stacking and acts as the leading electrolyte anion in the stacking dynamic. The Jaffe reaction has been successfully employed with concentrations between 5 and 0.5mM creatinine and experiments in the useful clinical range (0.1-2.0mM) are ongoing. To gain understanding of the stacking process, the computer simulation software SIMUL 5.0 was used to simulate the experimental work. SIMUL allows for frame-by-frame examination of the Jaffe reaction and stacking processes, providing information that cannot be obtained experimentally with a single on-line detector. The work with SIMUL suggests conditions for higher buffer conductivity to aid the stacking dynamic. Examination of the simulated ionic profiles leads to better predictions of the conditions to optimize the in-capillary Jaffe assay.

Support: National Science Foundation Grant DUE-1317446 and Bucknell Chemistry Department.

**NMR Investigations of Taurodeoxycholate Aggregation and Chiral Selectivity for Binaphthyl Compounds**

**Student:** Ross Pirnie  
**Supervisor (and any other co-authors):** Timothy G. Strein, David S. Rovnyak

**Short Description of work:** NMR is used to investigate bile salt aggregates. The structural dynamics of bile salt micelles and the basis for chiral selectivity in CE experiments is investigated using 1D $^1$H and 2D HSQC NMR.

Bile salts are naturally occurring amphiphiilic molecules with multiple stereocenters. Micelles formed from the aggregates of bile salts are capable of resolving chiral isomers of binaphthyl compounds through micellar electrokinetic capillary chromatography (MEKC). The complex intermolecular interactions that give rise to chiral selectivity in the bile salt micelle system, as well as the details of the structure and progressive nature of bile salt aggregation, are poorly understood. Here, intermolecular interactions of the bile salt taurodeoxycholate (TDC), which exhibits excellent chiral selectivity in MEKC, were studied with NMR and chiral probe molecule 1,1′-binaphthyl-2,2′-diyl hydrogen phosphate (BNDHP). Chemical shift analysis of $^1$H NMR spectra of TDC (0.0 – 60.0 mM) with either isomer of BNDHP revealed ring protons 4-7 constituted the binding edge of BNDHP, which is inserted into a hydrophobic binding pocket on the TDC micelle. The onset of large changes in $^1$H NMR chemical shift corresponding to a critical micelle concentration was observed in NMR spectra starting at 4.7 mM TDC. Chiral selectivity in the TDC host micelle was reported by carbon chemical shifts in heteronuclear single quantum correlation (HSQC) NMR experiments. Carbon 26 on the tail of the TDC molecule was shown to be especially chirally selective, suggesting the tail wraps back around to interact with the probe molecule. These data are consistent with a previously proposed model wherein bile salt monomers form skewed, antiparallel
dimmers, which preferentially bind the chiral isomers of BNDHP from opposite sides. These data also add important new information about chiral interactions of the flexible tail of TDC with guest analyte molecules.

Source of support for the work: NFS-RUI Grant 1153052

10,13-Nonadecadienoic Acid as a Substrate for Soybean Lipoxygenase and the F557V Mutant

Student: Morgan Price  
Supervisor: Dr. Charles H. Clapp

Lipoxygenases are enzymes that catalyze the incorporation of oxygen into polyunsaturated fatty acids. Soybean lipoxygenase is of particular interest, because of its similarities to mammalian lipoxygenases, which are involved in many cell interactions such as the inflammatory response and cancer. The active site of soybean lipoxygenase contains an iron atom that is near the center of the enzyme. Our current binding theory states that the substrate would enter tail first, with the carboxylic terminus at the surface of the enzyme. In the past, our group has prepared and studied a mutant of the enzyme we call F557V. In this mutant the phenylalanine group at position 557 has been replaced with a valine group. With linoleic acid, the enzyme’s normal substrate, and wild-type enzyme, almost all of the product is 13-hydroperoxy-9,11-octadecadienoic acid (13-HPOD). With the mutated enzyme, the percent of another compound, 9-hydroperoxy-10,12-octadecadienoic acid, jumps to 35%. It has been proposed that this product is formed by the substrate binding in an orientation that is reversed from the normal substrate binding mode. In the present work, we have shown that 10,13-nonadecadienoic acid, which has one more carbon than linoleic acid, is a substrate for both the wild type enzyme and the F557V mutant, and we are investigating the products of these reactions. The results will be used to test the reverse binding hypothesis.

Support: NSF-STEM Scholars Program and NSF-RUI CHE-1213262

Monitoring Gas Phase Kinetics Using FTIR Spectroscopy

Student: Ellie Siegfried  
Supervisor and co-author: Karen Castle and Kat Klein

The major objective of this research is to investigate the feasibility of using Fourier transform infrared spectroscopy (FTIR) spectroscopy to monitor the kinetics of interesting environmental gas phase reactions. Some important atmospheric reactions happen over time scales ranging from minutes to hours, therefore this simple technique may be useful.
This work has focused on understanding air samples around areas of acid mine drainage (AMD), which can contain high concentrations of sulfur compounds. Due to the mining process, minerals such as pyrite (FeS2) oxidize when exposed to air and water. This reaction forms sulfuric acid (H2SO4) and iron hydroxide (Fe(OH)3), an orange colored precipitate. Hydrogen sulfide gas (H2S) is then generated from sulfate reduction under certain conditions, which can later be oxidized to other sulfur containing compounds such as sulfur dioxide (SO2).

We are performing reactions similar to those that occur naturally in AMD regions in the laboratory. Na2S or ZnS is mixed with hydrochloric acid (HCl) in a 10-cm gas cell filled with air and the gas phase products are observed over time using FTIR absorption spectroscopy. As the reaction proceeds, the absorption peak corresponding to carbon dioxide (CO2) disappears as it is displaced by gas phase sulfur compounds. This enables gas phase kinetics of the sulfide-HCl reaction to be determined either by the loss of CO2 or by the formation of new gas phase products.

Support: Bucknell STEM Scholar Program funded by the National Science Foundation

**Title: Generation of Metallopolymers Through Protodeauration**

**Students: Kurt Vostal, Kevin Garcia, and Wade Heidel**

**Supervisor: Professor Robert Stockland**

Metallopolymers have been generated through protodeauration reactions using both conventional and microwave heating. A variety of monomers bearing a number of different functional groups were incorporated into the polymer chain in order to change the physical properties of the polymer. The presentation will outline the effectiveness of this approach to the preparation of metallopolymers with prescribed physical properties.

Source of Support: Petroleum Research Fund
Computer Science

Application of n-gram prediction and Brown’s Stages of Syntactic and Morphological Development to design augmentative and alternative communication for autistic children

Students: Robert Cowen, Marissa Mitchel CCC-SLP
Supervisors: Abby Hare-Harris Ph.D., and Brian King Ph.D.

The most recent data suggests that 1 in 68 children in the United States is diagnosed with autism spectrum disorder (ASD). Individuals with ASD exhibit impaired social communication skills, ranging from minor speech difficulties to complete lack of verbal communication. Even for children who are verbal, day-to-day communication can be a serious challenge, especially in social situations. With the advent of affordable personal computing devices such as smartphones and tablets, augmentative and alternative communication (AAC) applications, such as Proloquo2Go and Aacorn, have seen a rise in use by speech pathologists in the treatment of children with ASD. These applications typically provide children with a simple display of words which, upon selection, are spoken by the device to aid in communication. While these applications have proven useful, the user interfaces (UI) often lack the navigability necessary for children with ASD to use them efficiently, resulting in substantial learning-curves as well as significant decreases in word selection speed. The goal of our study was to develop an AAC application for Android tablets utilizing a word prediction model and streamlined UI in order to increase the communication rate and support the language development of children with ASD. The Android platform was selected due to its low cost and wide availability. Our application utilizes an n-gram model in order to predict the user's next target word. This decreases the number of keystrokes necessary to obtain the child's desired input. Our model is applied to corpora from the Child Language Data Exchange System (CHILDES), a database that contains thousands of transcripts of child speech. Transcripts were analyzed and organized by Brown's stages of child speech development. Our UI was developed with input from clinicians at the Geisinger Autism & Developmental Medicine Institute (ADMI) to be optimized for children with ASD. We plan on piloting the AAC app with patients from ADMI in the future.

1 http://www.cdc.gov/ncbddd/autism/data.html

Source of Support: James L. D. and Rebecca Roser Research Fund
Using Data Mining to Construct More Practical Weather Forecasting Models

Student: Jason Hammett  
Supervisor: Brian King

Weather is a phenomenal force, both breathtaking and violent. It affects all of our lives every day. The brunt of many jokes, weather forecasting is notoriously inaccurate. Developing models of the weather is not a simple task. It relies on thousands of numerical equations based on the physics of weather systems. Run by meteorologists, these models use enormous quantities of observations taken from thousands of weather stations across the world. Collection efforts have yielded a deluge of atmospheric and climate data. Even for local forecasting, there is too much data from too many sources for any meteorologist to fully analyze. The only players like government organizations or for-profit corporations capable of entering the field require massive supercomputers costing billions to run the numerical models. This is a fundamental problem requiring exploration of new techniques. Our work focused on creating accurate hyperlocal weather models that bypass the need for supercomputers by incorporating data mining and machine learning techniques, important, rapidly-evolving fields within computer science. Our research project took 2010 NOAA hourly weather data from land based stations in our geographical region and tested for the most effective and efficient algorithms and training sets. We set out with the goal of exploring the difficult nature of weather forecasting by using time series analysis.

Williamsport was our base forecast location, with tests comparing the effectiveness of using the regional data or solely this local data. Our experiments revealed the Support Vector Machine algorithm was the best performing algorithm at forecasting highly periodic weather data. It was highly adaptable to the changing seasons. The most effective implementation of the algorithm and most useful past weather training set is highly dependent on the nature of the weather attributes to be forecasted. Different models prove more accurate for different attributes such as temperature or pressure. When taking this into account, alternative techniques such as machine learning and data mining prove to be an excellent technique for forecasting meteorological data. These techniques have the potential to produce more practical local weather forecasters that reduce the immense cost and size of current, larger-scale atmospheric models.

Source of Support: James L. D. and Rebecca Roser Research Fund
Using Machine Learning to Automatically Predict Feature Representation on Sequential Data

Student: Son Pham  
Supervisor: Brian King

During the past recent years, Artificial Intelligence has pushed human beings further in the field of data analytic. A new AI technology called Deep Learning is now able to automatically detect features from a set of abundant data. This technology does not need any other human input beside the set of data itself to build an accurate representative model for the data it is given. For example, scientist only needs to plug-in human face raw data into the Deep Learning machine to automatically detect eye, nose, or mouth and differentiate human's face with the accuracy on par with human vision.

Audio and image detection have been the primary motivator for this technology. There have not been, however, significant application of this technology on other kinds of sequential data such as biological strings (DNA, protein, ...). Scientists have long struggled to find a meaningful classification model for these strings because these features have to be hand-engineered. These features usually contain an incredible amount of anomalies and exceptions as well as humans' bias. This create great opportunities for computer scientists to apply Deep Learning technology to automatically detect better and unbiased features and build a better classification model for these strings. Therefore, our project aims to apply Deep Learning to build a better classification model for Protein Secondary Structure. We will try to detect features on these strings and see if these features can be used in a meaningful way and help increase the accuracy of protein secondary structure prediction. Protein secondary structure is a good beginning position due to an abundance on protein secondary structure data. Successful application of Deep Learning on Protein Secondary Structure will lead to further expansion of the project into other fields of analytic such as meteorology, natural language process or finance.

Source of Support: Program for Undergraduate Research, The Dean’s Fund for Summer Undergraduate Research in STEM.
Geography, Public Policy

Changes in the National Flood Insurance Program Policy and the Implications for Lewisburg, PA*

Student: Greg Miller
Supervisors: Duane Griffin, Sam Pearson

The Biggert-Waters Flood Insurance Reform Act of 2012 and the Homeowner Flood Insurance Affordability Act of 2013 enacted significant changes to Federal flood insurance policies. These reforms completely altered the financial outlook for many property owners who are now faced with unnerving spikes in flood insurance premiums. Given their potential effect on property values, the impacts of these changes on towns like Lewisburg where approximately 40% of Borough structures are within the FEMA-designated flood zone, have the potential to be extreme. The situation is aggravated by the fact that the reforms in Biggert-Waters address problems predominantly relevant to coastal areas subject to building destruction by rushing waters, rather than river towns where flood waters rise slowly and damage, but rarely outright destroy, buildings within floodplains. The Lewisburg Neighborhoods Corporation (LNC) is in the process of analyzing these impacts to provide input to policymakers in hopes of making changes to the law when it comes up for reauthorization in 2017. Our goal was to aid the LNC in their preparation by using Geographic Information Systems (GIS) to conduct comprehensive spatial analyses of the Lewisburg floodplain. In conjunction with data supplied by Union County GIS, this research moves to model categories of flood depth and eventually mitigation costs to inform residents of floodplain structures of their options to relieve themselves of the impending financial burdens.

Support: Bucknell Institute for Public Policy
Emerging Scholars Interdisciplinary Summer Research Program

History and Wellness App Development

Students: Rajasri Alaparthi, Jiayu Huang, Henry Stann
Supervisors: Katherine Faull (Comparative Humanities Languages & Cultures & Linguistics), Joseph Tranquillo (Biomedical Engineering)

An interdisciplinary team of students from Bucknell University spent the summer working on the development of a smartphone application for the Health & Wellness Initiative. This new initiative brings Geisinger Health System in partnership with the National Park Service, PA Department of Conservation & Natural Resources, the Borough of Danville and the Montour Area Recreation Commission. This smartphone app reflects Geisinger’s interest in improving public health and wellness while reducing healthcare costs. At the same time, this App aims to generate public awareness in the historical culture of the area. The project includes a multi-year development of a self-tour and fitness smartphone application which will engage employees, patients and private citizens in activities that improve health through physical activity while also educating, rehabilitating and improving quality of life.

Students spent this summer making a proof of concept application on the iPhone to highlight the app’s key features. First the students began with a rough design of the app which included the map layers of the ‘pilot’ project areas. Historical data points were integrated into the map system through the creation of a personal database. The algorithm of accurately calculating the calories based on various user inputs was also factored into the app. The ‘pilot’ project areas are Montour Preserve, downtown Danville, and Geisinger campus.

Source of support for the work: Geisinger Health System, Mellon Digital Initiatives Grant

Fusion and Reconstructions: Translation Policies in China after the Cultural Revolution

Student: Tong Tong
Supervisor: Katherine Faull (Comparative Humanities Languages & Cultures & Linguistics)

The main aim of this research is to investigate the intercultural exchange between China and the rest of the world in the 1980s; specifically, why were certain non-Chinese authors translated into Chinese. I'm interested in conducting this research project because many
active and renowned contemporary authors in China have confessed that they are deeply influenced by world literature rather than by the traditions and classics of China. Also I chose the decade in 1980s because it is the so-called Golden Age for translation activities in China. This is an ongoing project with Professor Faull which was started in the Spring 2015. So far the database of all the literary works translated and published in one of the most influential literary magazines in China, Shijie Wenxue (World Literature) is established. In the following days, I’m working on the visualizations of the literary “data,” which include the use of geospatial and temporal analysis, network analysis and so on. This is a common way to explore research questions in the Digital Humanities and will definitely contribute to the rigor of the project.

Source of Support: Bucknell University (PUR program)

Text.0: Coding a Bridge from Archival Documents to Emotion Density Maps

Student: Ethan Vynalek
Supervisor: Kathryn Faull (Comparative Humanities Languages & Cultures & Linguistics)

Traditionally, within the humanities, the written word has been the only reliable link between the past and the present. Every medium, however, has its limitations; words convey information, but in a limited, narrative mode Any craftsman will tell you that a variety of tools are necessary to make a quality product - the same can be said of thorough text analysis; by employing technology to transform the written word into other analytical modes, we gain new insight and understanding. To demonstrate the power of document digitization and text encoding (specifically, XML compliant TEI) to aid comprehension, we encoded segments of the diary of an 18th century Moravian missionary (Martin Mack) linking emotions to the places they were experienced to produce an emotion-density gradient mapping of the area around the mission at Shamokin, the present day site of Sunbury. The resulting visualization helped us to identify the most commonly expressed sentiments at each locale visited or described by the author of the diary. The software package we created to perform the analysis has been made into a standalone analysis tool, to be made available for further research in the Digital Humanities and beyond. By creating an automated document analysis tool that successfully generated a series of meaningful emotion mappings, we have shown that this technology can collect data from historical documents, analyze that data to identify key trends and connections, and present the collected information as a map to enable non-linear examination of the contents of a document.
Environmental Studies

FEMA’s Community Rating System and Flood Management by Pennsylvania’s Small Communities: Federal Intent, Local Implementation

Student: Xueyang Zhang, Undergraduate Student
Supervisor: L. Donald Duke, Visiting Scholar

Flood mitigation planning, land use, and policy decisions in the US, largely made at the local government level, are profoundly influenced by multiple Federal and State policy instruments, regulatory requirements, and financial incentives. In Pennsylvania, among the most susceptible states to flood damage, about one-fourth of the population lives in rural or small communities, which are especially reliant on Federal and State programs. One federal program, the Federal Emergency Management Agency’s (FEMA’s) Community Rating System (CRS), offers flood-insurance rate reductions under the National Flood Insurance Program (NFIP) to residents of communities that voluntarily enact flood mitigation beyond the minimum standards. However, most eligible communities do not participate: of more than 21,600 US NFIP communities, only about 1,000 participate in CRS, and only 31 in Pennsylvania. Most of these reach the lowest levels: class 8 or 9 on a scale where 1 is most active and 10 is fewest. This research investigates several case-study small communities in Pennsylvania’s Central Susquehanna Valley, with the objective of identifying ways in which small communities participate in CRS; the extent to which CRS promotes flood mitigation; and ways in which CRS could enhance participation among small, rural communities. Research methods acquire and analyze publicly available information: CRS national and statewide data to characterize activities by communities nationwide, especially Pennsylvania participants; and routine reports and re-certification studies by selected case study communities for in-depth analysis of their CRS activities, and reasons for their limited participation. Preliminary findings indicate municipalities in the target region employ a range of flood mitigation strategies, differing widely from one another; these activities are captured only to a limited extent by CRS documentation; and they seldom undertake new or more-intensive activities for the purpose of gaining in CRS ratings. The CRS application and reporting paperwork is seen as highly burdensome and the rewards to municipalities seen as limited. Preliminary recommendations suggest that reducing reporting and documentation, and increasing FEMA personnel support to communities, may increase the number of participating communities and may incentivize them to more actively seek out and implement strategies of the kinds recommended by CRS.

Key terms: Flood management, Water resources, Rural communities, Urban planning, Small municipalities, Environmental policy
Mechanical Engineering

Analysis of Stiffness Degradation in Additive Manufactured Parts During Cyclical Tensile Loading

Student: Kellen Haile  
Supervisor: Professor Constance Ziemian  
Collaborator: Maryvivian Okwara

Layered acrylonitrile butadiene styrene (ABS) dogbone specimens, with a variety of different fiber orientations, have been fabricated by an additive manufacturing process known as fused deposition modeling (FDM). Eleven different fiber orientations or meso-structures were produced, including seven unidirectional and four cross-ply configurations. Monotonic tension tests were first run to determine the mean ultimate tensile strength (UTS) associated with each meso-structure, for use in subsequent cyclical fatigue testing. Computational algorithms were developed and written in MATLAB to analyze the results and compute the effective elastic moduli (E) and the secant fatigue moduli (F) of each ABS specimen at each cycle of testing. Data have been analyzed to assess how the degradation of both E and F are affected by specimen meso-structure. Results suggest that the rate at which stiffness (E and F) decreases is a function of both meso-structure and the maximum percent UTS of the fatigue test. Stiffness degradation results are currently being used in the development of an empirical model of fatigue life. Additional physical testing is also underway to allow for the future analysis of the residual strength degradation that occurs during cyclical tension fatigue.  
Source of Support: Bucknell STEM Scholars Program

Physics & Astronomy

Forward Modelling of Brown Dwarfs

Student: Dunni Adenuga  
Supervisors (and any other co-authors): Katelyn Allers & Jack Gallimore

Short Description of work: Brown dwarfs are a recent discovery. To learn more about their properties, we use forward modelling of infrared spectra to measure their radial and rotational velocity. We fit to the same data observed in different spectral orders (wavelength bands) to assess the systematic uncertainty. We use DREAM(ZS), a Markov Chain Monte Carlo based algorithm, to fit the models to the brown dwarf spectrum. We
find that we are able to determine radial velocities to a statistical precision of about +/- 1 km/s and rotational velocity to a statistical precision of +/- 1 km/s. By comparing the results of different spectral orders, we find that there are systematic uncertainties of order +/- 3 km/s.

Source of support for the work: Issac J. Tressler Fund for Astronomy

**Observing the Motion of Bacteria in a Two-Dimensional Fluid Flow: Do Wild Bacteria and Smooth Swimmers Encounter Reaction Front Barriers?**

*Students: Minh Doan and Katie Lilienthal*

*Supervisor: Tom Solomon*

We observe the motion of self-propelled particles in a two-dimensional fluid flow to find evidence of barriers as predicted by the Burning Invariant Manifold Theory. The flow configuration of two adjacent vortices is generated by a cross shape polydimethylsiloxane (PDMS) microfluidic channel. Two types of self-propelled particles, wild type and mutated smooth swimming bacteria, are used to compare and contrast.

Source of support: NSF STEM Grant #DUE-1317446, Solomon NSF RUI grant

**Finding Evidence of Barriers for Reaction Fronts Propagating in Three-Dimensional Fluid Flows**

*Students: Minh Doan and Katie Lilienthal*

*Supervisor: Tom Solomon*

We are observing reaction fronts propagating through three-dimensional fluid flows. The goal of this experiment is to find evidence of barriers and observe the structure of the barriers. The flow is a nested vortex chain and single vortex chain. We use the excitable Belousov-Zhabotinsky chemical reaction to produce the reaction fronts. Our results are interpreted by use of the Burning Invariant Manifold Theory.

Source of support: NSF STEM Grant #DUE-1317446, Solomon NSF RUI grant
Measuring Reaction Front Propagation in Vortex Dominated Flows --- The Effect of Reaction Barriers on Front Propagation Speed

Student: Joseph-John Simons  
Supervisor: Tom Solomon  
Collaborators: Laura Skinner, John Mahoney (UC Merced), Kevin Mitchell (UC Merced)

Reaction fronts are common phenomena in nature that play a role in diverse systems. These fronts in vortex dominated flows can produce invisible barriers that restrict movement. The key question is how these barriers affect the overall front propagation speed. We use Burning Invariant Manifolds (BIMs) to explain these barriers, and in accordance with the BIM theory, we adjust the placement of these barriers to observe their effect on the overall reaction front propagation speed.

Source of support: NSF STEM Grant #DUE-1317446, #PHY-1156964, #DMR-1361881

Adaptations in Dynamic Vascular Networks

Student: Sean McMahon  
Supervisor: Jim Baish (Biomedical Engineering)

We study adaptations in blood vessel networks, particularly how these networks respond to damage in order to maintain adequate distribution of oxygen. Our primary case study is a section of an experimentally observed arterial network in a mouse. Using the diameters, lengths and relative directions of flow obtained from intravital microscopy, we implement a Monte Carlo simulated annealing process to recover the unknown pressures at the boundaries of the observed network as well as the uncertainties in the recovered pressures. These boundary pressures give us a basis on which to study the redistribution of flow throughout the network if a blood vessel near the center of the observed network is damaged and is no longer able to support flow. To study the effects of these damaged central vessels in a larger scale network, we create synthetic networks similar in structure to the experimental network and observe the relationship between the changes in a vessel’s flow and its proximity to the damage. We find that the density of closed loops in the network plays a critical role in determining the resilience of vascular networks to damage. Our study provides insights into stroke, heart disease and vascular tumors.

Source of support: Department of Physics and Astronomy
Spectroscopic Confirmation of Young Brown Dwarfs

Student: Teweldeberhan Misghina  
Supervisor Name: Katelyn Allers

The goal of our research is to do spectroscopic analysis of brown dwarfs. We start by reducing the spectra of candidate brown dwarfs using an IDL dwarf with spectra of known brown dwarfs from the IRTF library. For example, we select one of our brown dwarfs which is a candidate member of the Tucana-Horologium Association whose age is estimated to be 41 Myr (Kraus et al. 2014). By the using effective temperature of our brown dwarf. Finally, we used the effective temperature and age, and the model evolutionary tracks to estimate the mass of our brown dwarf.

Source of support: Physics and Astronomy NSF REU Grant #PHY-115964

Real-time Optimization of an Ion Optical Beamline

Student: Zach Schillaci  
Supervisor: Matthew Amthor  
Co-authors: M. Portillo, Facility for Rare Isotope Beams

We have developed an experimental approach to automatically adjust multiple electrostatic and/or magnetic elements on an ion optical beamline, while analyzing the profile of the beam on a detector at the image point, until an optimal tune is found. This approach dramatically simplifies beamline tuning, thus allowing more efficient use of experimental equipment; ensures a more optimal tune is found, providing a more focused beam spot without a significant loss of beam transmission; and will allow the development of specialized optical tunes based on the needs of any given experiment. The optimizer is based on the particle swarm optimization method, in which a swarm of particles is initialized in an n-dimensional space, with the position of each swarm particle as an n-dimensional position vector representing a particular tune of the n electric or magnetic elements along the beamline being optimized. At each system iteration, the beamline is adjusted to match a given setting and the image of the beam spot is analyzed to measure the quality of that setting. The quality measure is then sent back to the optimizer to inform its future progress. The D-Line system at the National Superconducting Cyclotron Laboratory at Michigan State University is an ideal beamline for the first test of the optimizer, thanks to its relatively low number of rapidly-tunable electrostatic elements. The optimizer approach was first developed using Monte Carlo simulations based on an ion optical model of the D-Line. Then the approach was tested directly on the D-Line in several real-time optimization runs with 30 kV beams of Rb and other species. The initial experiments demonstrate the ability of the optimizer to focus the beam while preserving transmission, ultimately halving the x and y RMS of the beam spot relative to that produced through a manual tuning of the elements. With further research we plan to generalize the approach to work on any given beamline consisting of
any number of electrostatic and/or magnetic elements, including particularly for higher order tunes of fragment separators currently under operation or development around the world (e.g. the A1900 at NSCL, BigRIPS at RIKEN, S3 at GANIL, and ARIS at FRIB).

This research was made possible through NSF REU Grant #PHY-1156964, Department of Physics and Astronomy at Bucknell, and NSF Grant #PHY-1102511, National Superconducting Cyclotron Laboratory at Michigan State University.

**Finding Brown Dwarfs in Ophiuchus via Proper Motion**

**Student:** Jake Simon  
**Supervisor:** Katelyn Allers

In the study of young stellar objects, we attempt to identify possible candidates members of Ophiuchus via their proper motion. Images from the Spitzer Space Telescope are processed by extracting the sources, then running a battery of reductions to determine their proper motions. If our models we generated using the Besançon Galaxy model are correct, we should expect an appreciable difference between the proper motion of Ophiuchus members and the background stars, allowing us to classify those members as brown dwarf candidates.

**Source of support:** Allers STSI Survey of the Brown Dwarfs

**Observing Reaction Front Barriers in a Vortex Flow**

**Student:** Laura Skinner  
**Supervisor:** Tom Solomon

From past experiments we have been able to see barriers that impede reaction fronts in vortex dominated flows. This behavior can be characterized by a theory of burning invariant manifolds (BIMs). Previously we observed barriers in time independent flows. Our current experiment aims to extend the BIM approach to time dependent flows. We are looking at the pinning of reaction fronts in vortex flows in the presence of an imposed wind. The addition of time dependence can cause the transition to unpin.

**Source of support:** Physics and Astronomy NSF REU Grant #PHY-115964
Infrared SED Decomposition of Active Galactic Nuclei

Student: Emily Stump
Supervisor: Jack Gallimore

We developed a code, clumpyDREAM, to decompose the spectral energy distributions (SEDs) of 83 active galactic nuclei (AGNs). We used the parameters obtained from this decomposition to compare the characteristics of the obscuring medium (dusty tori) surrounding black hole accretion disks of Type 1 and Type 2 Seyfert galaxies. In the simplest version of AGN unifying schemes, the only parameter that should distinguish Type 1 and Type 2 AGNs is the torus inclination. We find, however, that Type 2 galaxies from this sample have overall larger tori, both in angular scale height and radial extent, suggesting a possible intrinsic difference in the structures of Type 1 and Type 2 AGNs.

Source of support: Physics and Astronomy NSF REU Grant #PHY-115964

Psychology

Effects of Being Forgiven on Empathy and Acceptance of Responsibility

Student: Vincent Ancona
Supervisor: Dr. Kimberly Daubman

Psychologists have considered understanding the relationship between forgiveness and psychological well-being to be fundamental for victim rehabilitation. Because of this, much research has been conducted on the effects of victims forgiving offenders, specifically on the critical role of forgiveness as a vehicle for overcoming negative feelings and regaining self-respect. However, considerably less research has examined the effects of being forgiven on the offender. The present study recruited one hundred participants from all over the world via the Mechanical Turk marketplace and investigated the effects of forgiveness on offenders. This was accomplished by measuring the relationship between being forgiven or not forgiven by their victims and four dependent variables: empathy, victim blame, personal accountability, and desire to maintain future contact with victims. It was predicted that receiving forgiveness from victims would increase the offender’s empathy for the victim, increase their personal accountability for the offense, decrease their blaming of the victim, and increase their desire to maintain future contact with the victim. It was also predicted that each of these four effects would be mediated by perceived social acceptance. The analysis showed that transgressors reported more empathy and increased desire to maintain future contact
with their victims when forgiven than when not forgiven, with social acceptance as a reliable mediator in both cases. Results further yielded that there was no statistically significant increase in personal accountability or decrease in victim blame as a result of being forgiven. This study is part of a growing body of research on the effects of forgiveness on offenders. Future studies should examine the relationship between forgiveness and empathy, personal accountability, victim blame, and desire to maintain contact with victims using a larger and more diverse subject pool. Future studies should also deploy novel methodologies to better determine cause and effect relationships between forgiveness and the aforementioned dependent variables. This project will contribute to future research on similar topics.

Source of Support: This work was funded by the Emerging Scholars in Psychology (ESP) program within Bucknell University’s Department of Psychology.

**Testosterone reduces alcohol consumption in the context of exercise**

**Student:** Zach Kozick  
**Supervisor:** Judy Grisel;  
**Coauthors:** Megan Summers, Todd Nentwig, Colleen McGonigle, & Barrie Rogers

A range of genetic and environmental factors, one of which is stress, impacts EtOH consumption. Research indicates that males exhibit lower alcohol consumption and less stress vulnerability than females, phenomena suggested to be hormone dependent. Our research is aimed at understanding these sex differences by exploring the role of testosterone in voluntary oral EtOH consumption. We hypothesize that castrated males will consume more EtOH compared to sham-operated, or naïve mice. In Experiment 1, castrated, sham, and naïve C57BL/6J males were allowed access for 2 hr a day to 20% ethanol, in addition to 24 hr access to food and water. We measured consumption and preference for the EtOH solution. In Experiment 2, mice had the same 2 hr access to EtOH, along with the possibility of voluntary exercise provided by an activity wheel. The running wheel was available all the time, except on alternating test days when the wheels were locked beginning one hour prior to EtOH availability. Our results indicate that the effects of testosterone on drinking were context-dependent. There were no effects of testosterone on voluntary consumption in Experiment 1; naïve, sham and castrated males drank similarly. However, when the mice had an opportunity to engage in voluntary running on a home cage activity wheel, intact males drank less alcohol compared to castrated males. These results indicate that testosterone is involved in alcohol consumption in an exercise-dependent manner. Our data suggests that drinking can be mitigated by exercise in male mice, but testosterone plays a critical role in this effect. Better understanding the sex-dependent factors affecting alcohol use and abuse will promote more effective treatment and prevention of alcoholism.

Support: NIH grant #R15 AA022506, Douglas K. Candland Undergraduate Research Fund, and STEM Scholar Program funded by the National Science Foundation.
Ovarian hormones promote vulnerability to effects of exercise restriction

Student: Colleen McGonigle  
Supervisor: Judy Grisel  
Coauthors: Barrie Rogers, Megan Summers

Stress is a psychological state correlated with behavioral and physiological changes reflecting some perturbation of homeostasis. Among its multifarious effects is an increase in voluntary alcohol consumption. The interaction between stress responses and alcohol consumption is sex-dependent in part and its mechanisms are poorly understood. Our general research is aimed at helping to clarify the connection between stress and drinking; the present study was designed to explore the effect of ovarian hormones on this relationship. Prior studies in our lab suggested that females are more susceptible to the negative reinforcing effects of alcohol than males, and therefore find it more rewarding under stressful conditions (Piza-Palma, et al., 2014). Our hypothesis in the present experiment was that the females’ increase in stress sensitivity is mediated by gonadal hormones. In order to test this, 8 ovariectomy, 8 sham-operated, and 8 naïve female C57BL/6 mice were given continuous access to an activity wheel, food, and water in their home cage. Following a baseline period in which they were acclimated to the housing conditions as well as 2hr daily access to 20% EtOH, we manipulated access to the activity wheel in order to induce stress. On alternating days the running wheels were placed in a locked position, beginning 1hr before alcohol availability. In intact females there was a clear increase in drinking levels in response to a locked running wheel versus an unlocked wheel, as we expected. This effect was not observed in ovariectomy females. That is, alcohol consumption in ovariectomy females did not differ depending upon access to the running wheel, suggesting that ovarian hormones contribute to the effect of stress on drinking. Overall alcohol consumption between sham-operated and OVX females did not differ, suggesting that estradiol, and/or its derivatives, influence drinking in response to stress, rather than overall alcohol consumption. These data address an important yet understudied area of alcoholism research, where females have traditionally been underrepresented. A better understanding of the source of sex difference in alcohol consumption will help address the increasing use and abuse of this drug by women.

Support: NIH grant #R15 AA022506, Douglas K. Candland Undergraduate Research Fund and STEM Scholar Program funded by the National Science Foundation.
The Effect of Touch on Infant Word Learning

Students: Haley Tighe and Sarah Och
Supervisor: Ruth Tincoff

Objective. At six months of age infants begin to understand names and body part words. This presents the question of how infants are able to learn these words? Body part words, unlike names, do not often occur in isolation when parents are talking to infants.

Background. Previous research shows how touch cues help infants find words in the talk they hear, a process called word segmentation and a key step to word learning. Further research shows that when teaching infants word games, caregivers initiate informative touches that might naturally help infants segment these early words.

Hypotheses. In the present study, we hypothesize that if touch is relevant for infants’ initial understanding of early words, then infants feeling touch while listening to a word pattern will map the word to the body part where the touch was felt. In contrast, infants should not map word patterns that are not paired with touch to body parts.

Method. We tested these hypotheses using an Exposure + Test experimental design with 4- to 6-month-old and 9- to 11-month-old infants. Infants were exposed to a stream of syllables. One string of three syllables was always paired with a touch to the body (e.g., elbow). A different three syllable string was paired with a touch only once. The speech-touch hypothesis predicts that, when tested for learning the mapping between the syllable string and the body part that infants in the Always Touch condition should look longer at a video of a person’s elbow than to a distractor video. Infants in the One Touch condition should not show learning.

Results & Conclusions. Coding of the direction and duration of the infants’ looking times is in progress.

Source of Support. Program of Undergraduate Research Fellowship and the Bucknell Psychology Department

Measuring Grit in Capuchin Monkeys (Cebus apella)

Student: Niara Nelson
Supervisor: Regina Gazes

Grit is defined as perseverance and passion for long-term goals, working strenuously towards challenges, and maintaining effort and interest over time despite failure, adversity, and plateaus in progress (Duckworth et al., 2007). In humans, grit is positively correlated with major accomplishments that require intensity of effort, consistency in direction, and a large time commitment, such as achieving a leadership position in college or completion of a military training program. Like humans, individual monkeys differ in their success in social situations and in cognitive tasks. If traits measured by grit, such as perseverance and maintaining effort despite difficulties are integral to success in humans, these traits may also be related to success in monkeys. We designed a task to
measure these traits in monkeys by presenting the individuals with a situation in which they were motivated to complete a goal that was impossible to complete. Monkeys were presented with a sealed tube filled with grapes (a preferred food item). Monkeys tried to obtain the grapes (goal), but the tube could not be opened, creating difficulty for achieving this goal. Perseverance and persistence were measured by recording the amount of time during a 10 minute trial each animal spent interacting with the tube and by the number of unique strategies each monkey employed in their attempt to reach the goal. If this new method for testing grit in monkeys is successful, it will provide a test to help us understand what factors contribute to individual differences in animals.

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