# Summer Science Institute Research Symposium 2021

Wednesday, July 21st
Virtual Symposium
University of Mary Washington
VIRTUAL SYMPOSIUM

**Explanation of Poster Session:** Each link goes to a single poster. To "walk around and visit a poster" you click on the link and the poster and presenter will be there. After that, please treat it as though you were actually at the poster. If you wish to visit another poster, just leave that zoom meeting and click on another link. To get a better view of the posters, the PDFs for each poster is linked below the zoom link.

# Summer Science Institute
# Research Symposium 2021

## Schedule of Events

**OPENING COMMENTS** **9:00**

**MORNING ORAL PRESENTATIONS** **9:05 – 10:45**

**Zoom Link:** https://umw-sso.zoom.us/j/83043541797?pwd=djNzRXdZUDFpTEpPdmkrTFRVRHJIdz09

9:05 SARAH KERNER
**Fluctuating Asymmetry as a Bioindicator of Environmental Stress from Urbanization in the Rappahannock Watershed Area**
Advisor: Dr. Bradley Lamphere

9:20 HANNAH HARRIS
**Synthesis of the Stereoisomers of DEHP and Its Oxidative Metabolites**
Advisor: Dr. Davis Oldham

9:35 TREVOR DRINKWATER
**Analytical and Numerical Analysis of the SEIRP Model for Covid-19**
Advisor: Dr. Leo Lee

9:50 – 10:00 BREAK

10:00 DRAKE RICHMOND
**Rotational and Vibronic Couplings in Molecular Dynamics**
Advisor: Dr. Varun Makhija

10:15 ANDREA WALTRIP
**Locating Transgene Insertion Sites in Drosophila Myotonic Dystrophy Type 1 Models**
Advisor: Dr. Ginny Morriss

10:30 RINA MURKASKI
**Assessing the Impacts of Neonicotinoid Pesticides on the Viability, Biomass, and Behavior of the Earthworm (*Eisenia fetida*) Using an Agar Medium**
Advisor: Dr. Tyler Frankel

## MORNING POSTER SESSION 10:45 – 12:00

GRACE HOLCOMB

**Endothelial Tube Maintenance in a HUVEC cell Model for Myotonic Dystrophy Type 1**

Advisor: Dr. Ginny Morriss

Zoom link: https://umw-sso.zoom.us/j/89029147108?pwd=ZGpBNk1IZzNURXJZSlkrb0RkODBlQT09

KAYLA BOTTO

**Genomic Similarity to Predict Infection in Bacteriophages**

Advisor: Dr. Lynn Lewis

Zoom link: https://umw-sso.zoom.us/j/88018748638?pwd=NHZpcVBpNE4xV2prNnlCTnd4Um94Zz09

HANNAH LEE

**The Role of PGAM5 in Apoptosis in Kinetoplastids**

Advisor: Dr. Swati Agrawal

Zoom link: https://umw-sso.zoom.us/j/81136023013?pwd=L09raXkvOXdHTUNhNU9aamN2MmhYQT09

SHREYA MURALI

**Apoptosis Induction in Jurkat T Lymphocytes by Proton Pump Inhibitors**

Advisor: Dr. Randy Reif

Zoom link: https://umw-sso.zoom.us/j/84465630985?pwd=a3hyODh3SXVEVmc5Y0lNdEl2L1hQZz09

ZOE RAFTER

**Angular Momentum Coherences in Vibrational Molecular Dynamics**

Advisor: Dr. Varun Makhija

Zoom link: https://umw-sso.zoom.us/j/87202792475?pwd=N3EycEZxQjhJczVJM0JWVTZmT1RGQT09

ALEXIS KOCHANSKI

**Bootstrapping Training Data for a Political Polarization Classifier**

Advisor: Dr. Stephen Davies

Zoom link: https://umw-sso.zoom.us/j/84978770786?pwd=emdZU1lNUk1WL243Q1p4Zlk1Qzlrdz09

CATHERINE CROWELL

**The Effects of Coal Ash Concentration on the Development, Hatching Rate, and Reproduction in *Planorbella duryi***

Advisor: Dr. Tyler Frankel

Zoom link: https://umw-sso.zoom.us/j/86412285876?pwd=eDBnekQzZkxUSUd2WDBJdXlqYXBwQT09

**LUNCH** **12:00 – 12:30**

**AFTERNOON ORAL PRESENTATIONS** **12:30 – 2:15**

**Zoom Link:** https://umw-sso.zoom.us/j/83043541797?pwd=djNzRXdZUDFpTEpPdmkrTFRVRHJIdz09

12:30 MADELINE KILLIAN
**Rotational Dynamics of Asymmetric Molecules**
Advisor: Dr. Varun Makhija

12:45 ABIGAIL DELAPENHA
**Understanding the Role of the Bax-1 Inhibitor and AATF Genes in Apoptosis of Kinetoplastid Parasites**
Advisor: Dr. Swati Agrawal

1:00 SOPHIA WELDI
**Assessing the Impacts of the Common Deicing Agent NaCl on the Viability, Embryonic Development, and Behavior of the Freshwater Snail *Physa acuta***
Advisor: Dr. Tyler Frankel

1:15 – 1:25 BREAK

1:25 VERONICA CAGLE
**Using Machine Learning to Identify Political Polarization on Social Media**
Advisor: Dr. Stephen Davies

1:40 RAMSEY COTTON
**Temporal Dynamics of the Intrinsic Pathway of Apoptosis via Doxorubicin Induction**
Advisor: Dr. Randy Reif

1:55 RACHEL MYRICK
**Effect of Social Hierarchies on Exercise in Social Mice**
Advisor: Dr. Parrish Waters

## AFTERNOON POSTER SESSION 2:15 – 3:30

ALEX FERNANDEZ

**Morphological Changes in Non-Native Fish Species Influenced by Differences in Upstream and Downstream Habitats**

Advisor: Dr. Brad Lamphere

Zoom link: https://umw-sso.zoom.us/j/89029147108?pwd=ZGpBNk1IZzNURXJZSlkrb0RkODBlQT09

ABIGAIL VORSTEG

**Myokine Expression in a Myotonic Dystrophy Type 1 Cell Culture Model**

Advisor: Dr. Ginny Morriss

Zoom link: https://umw-sso.zoom.us/j/88018748638?pwd=NHZpcVBpNE4xV2prNnlCTnd4Um94Zz09

KARISSA HIGHLANDER

**Synthesis of Indazole Inhibitors of KasA, a Vital Enzyme of *M. tuberculosis***

Advisor: Dr. Davis Oldham

Zoom link: https://umw-sso.zoom.us/j/81136023013?pwd=L09raXkvOXdHTUNhNU9aamN2MmhYQT09

DOCIA ATANDA

**Using Additive Manufacturing To Increase Reproducibility In A Packed Bed Column**

Advisor: Dr. Sarah Smith

Zoom link: https://umw-sso.zoom.us/j/84465630985?pwd=a3hyODh3SXVEVmc5Y0lNdEl2L1hQZz09

LYRA WINTERS

**Paleoclimate analysis using growth bands and stable isotopes from mid-to-late 1700s Stratford Hall oysters**

Advisor: Dr. Pam Grothe

Zoom link: https://umw-sso.zoom.us/j/87202792475?pwd=N3EycEZxQjhJczVJM0JWVTZmT1RGQT09

CAITLIN HOLT

**A Numerical Study of COVID-19 using the SVIR Model**

Advisor: Dr. Leo Lee

Zoom link: https://umw-sso.zoom.us/j/84978770786?pwd=emdZU1lNUk1WL243Q1p4Zlk1Qzlrdz09

## CLOSING COMMENTS AND AWARDS CEREMONY 3:45

**Zoom link:** https://umw-sso.zoom.us/j/83043541797?pwd=djNzRXdZUDFpTEpPdmkrTFRVRHJIdz09

**Fluctuating Asymmetry as a Bioindicator of Environmental Stress from Urbanization in the Rappahannock Watershed Area**

Sarah Kerner, Environmental Science Department
Faculty Advisor: Dr. Bradley Lamphere, Biology Department

Urbanization increases the environmental stress of a stream's ecosystem due to runoff of effluents and excess nutrients, which is important in understanding how humans are impacting the waterways and its organisms. Here it is tested whether fluctuating asymmetry (FA), the random deviations between normally bilateral morphology, could serve as an indicator of urbanization stress in a common native fish, the Bluegill (*Lepomis macrochirus)*. The hypothesis is that as urbanization increases in a watershed, then the FA increases from stressful living conditions not within optimal tolerance zones causing developmental errors. FA was quantified by comparing 3 photos of the left and right sides of fish then analyzing the data using geometric morphometric software (TPS, SAGE). The PCA reduces the dimensionality, increases the interpretability, and computes the variances for the morphologic asymmetry. Urban land use at the 10 sample sites, as determined from ArcGIS Pro, varied between 4.7% and 68.9%. A biplot showed that FA at each stream was different at all 10 sites with vectors showing strong loadings with landmarks at the caudal peduncle, bottom of the top lip, anterior of the eye, first nostril, posterior of the pelvic fin, joint of the lip, bottom of the operculum, and second nostril. There is a unimodal response with peak of PC1 averages in intermediate urban use. This could be from higher stress environments killing off individuals who have high FA and leaving behind robust fish with higher tolerance and low FA.

**Synthesis of the Stereoisomers of DEHP and Its Oxidative Metabolites**

Hannah Harris
Faculty Advisor: Dr. Davis Oldham

Di(2-ethylhexyl) phthalate (DEHP) is a chiral molecule used to add flexibility to plastics that can leech from many commercial products. Its primary metabolite, MEHP, and several oxidative metabolites have been linked to endocrine disruption and other adverse health effects in animals and humans. Differences in the toxicity of the stereoisomers are not well studied. In order to synthesize (R,R)-DEHP **(1)**, 2-ethyl-1-hexanol was reacted with vinyl acetate and Amano Lipase PS in dichloromethane at 0˚C until (R)-2-ethyl-1-hexanol **(2)** with 97:3 e.r. by chiral GC-FID analysis remained. 2-ethyl-1-hexyl acetate **(3)** was also obtained from this reaction. **(2)** was refluxed with phthalic anhydride and pyridine, yielding (R)-MEHP **(4)**. **(4)** was further esterified with **(2)** resulting in (R,R)-DEHP **(1)** (35% total yield). **(3)** was hydrolyzed to recover (S)-2-ethyl-1-hexanol **(5)** (75:25 e.r.) and again resolved using immobilized Amano Lipase PS to yield **(5)** (96:4 e.r.) after hydrolysis. The same procedure was followed to produce (S)-MEHP **(6)**, (R,S)- DEHP **(7)** (8.5% total yield, 95:5 e.r.) and (S,S)-DEHP **(8)** (32% total yield). To synthesize 2cx-MMHP **(9)**, one of DEHP's oxidative metabolites, an enolate alkylation was performed with methyl hexanoate and allyl bromide to form 2-allylhexanoate **(10)** which was reduced to 2-allyl-1-hexanol **(11)** by $LiAlH_4$. **(11)** was esterified with phthalic anhydride to yield mono(2-allylhexyl) phthalate **(12)** which was oxidized to form **(9)** (17% total yield). Future work will focus on synthesizing two other oxidative metabolites, 5-cx MEPP and 5-oxo MEHP, as well as their enantiomers as a means for determining if a chiral component to phthalate toxicity is present.

**Analytical and Numerical Analysis of the SEIRP Model for Covid-19**

Trevor Drinkwater
Faculty Advisor: Dr. Lee

We apply the Susceptible-Exposed-Infected-Recovered-Passed (SEIRP) model, a system of 5 ordinary differential equations, to Covid-19 Coronavirus epidemics and analyze this model both analytically and numerically. Numerical approximation methods are used to investigate the trends of the epidemic in the United States, India, and Virginia; furthermore, exact solutions are found from two simplified versions of the model. Investigating the trends of Covid-19 provides insight into the future of its presence in these regions. For the numerical analysis, various numerical approximation methods are constructed into MATLAB codes to approximate a solution to the model. Then, parameter values are either assumed based on the safety measures taken or estimated using confirmed collected data. The results provide an illustrative picture of the declining trend of infected populations with Covid-19 in all three studied regions. For the analytical analysis, an approach is used to solve the two simplified models. This involves solving for one of the dependent variables implicitly, then integration and various substitutions are made to have all equations as a function of that dependent variable. Therefore, both models have a solution in the form of an implicit equation. These solutions showcase how the exposed population, pre-symptomatic and asymptomatic individuals, affects the spread of Covid-19 without the influence of symptomatic individuals.

**Rotational and Vibronic Couplings in Molecular Dynamics**

Drake Richmond
Faculty Advisor: Dr. Varun Makhija

This project focuses on the interplay of interactions in Molecular Dynamics (MD). MD is the study of the behavior of an isolated molecule immediately after energy from incoming light is transferred into the system. This light-matter interaction is the very beginning of many natural processes, such as vision and photosynthesis. This energy is absorbed by the orbiting electrons, inducing electronic motion. The electrons then exchange energy with the nuclei of the molecule, causing it to vibrate and rotate. This project accounts for all three types of motion in an excited state of ammonia (NH3), and aims to computationally simulate ensuing molecular motion after excitation. A previous study exists in the same excited state of NH3 in which vibrational motion was frozen. Accounting for vibrational states leads to a vibrational and electronic (vibronic) state coupling. The results indicate that these vibronic couplings play a significant part in overall dynamics, and are strongly dependent on the orientation of the molecule, which varies in time as it rotates. This coupling is related to a molecular symmetry-distorting effect (Jahn-Teller Effect) in certain states, which implies that quantum entanglement between the nuclei and electrons may have an influence on overall molecular motion. Further calculations aim to investigate the degree to which the effects of entanglement are realized, and how it varies over time.

**Locating Transgene Insertion Sites in Drosophila Myotonic Dystrophy Type 1 Models**

Andrea Waltrip
Faculty Advisor: Dr. Morriss

Myotonic Dystrophy Type 1, DM1, is a muscle wasting disorder that is the result of expansion of CTG repeats in the *DMPK* gene on the 19$^{th}$ chromosome in humans. *Drosophila melanogaster,* fruit flies, are used as model organisms to study DM1 and determine possible treatments. CTG-repeat containing transgenes, have been inserted into *Drosophila* to model DM1. There is currently no published research showing where these DM1 transgenes have been inserted into the fruit fly genome. Knowing where the transgenes have been inserted is crucial information to have when performing genetic crosses. We are using classical genetic approaches to identify onto which chromosomes the DM1 transgenes have been inserted. Genetic crosses using the GAL4-UAS system to drive expression of the repeat expansions were performed such that phenotypic ratios of resulting $F_2$ offspring will differ depending on which chromosome the transgene is localized. The phenotype being assessed will be flight capability, which previous publications have shown is defective in DM1 flies. To test flight ability, we built a flight cylinder and will measure the flight distance of the DM1 and control flies. An initial fly flight test was run with wild type flies to have a baseline and to optimize methods for testing the transgenic flies. Preliminary results have shown that some flies with a skeletal muscle-specific driver expressing 480 repeats showed limited flight ability. Continued flight tests will be conducted to determine the best driver of the repeat expression.

**Assessing the Impacts of Neonicotinoid Pesticides on the Viability, Biomass, and Behavior of the Earthworm (*Eisenia fetida*) Using an Agar Medium**

Rina Murasaki
Faculty Advisor: Dr. Tyler E. Frankel

Recently developed pesticides, such as thiamethoxam and sulfoxaflor, are commonly utilized in the United States based on their high efficacy and improved target toxicity for pest species. However, recent studies have found harmful effects on beneficial insects including the honeybee (*Apis mellifera*). Despite earthworms being agriculturally desirable, there are minimal studies on the effects of these insecticides on their viability, physiology, and behavior. As natural and artificial soil have complex chemical relationships with contaminants, an artificial agar matrix serves as a possible habitat and exposure medium for toxicology assays. Various concentrations (0, 12.5, 25, 50, 100, and 200 ug/L) of either thiamethoxam or sulfoxaflor were homogenized into 2.0% reconstituted agar. Earthworms were individually massed and added to glass vessels containing 50mL of the treatment agar (n=4). Body mass and locomotor behaviors were recorded after 14-days and quantified using the behavioral analysis software, ToxTrac (v2.95). While this experiment is ongoing, we expect to observe a dose-dependent decrease of biomass and mobility in earthworms with both pesticides, with more severe effects in the sulfoxaflor treatments. These results will 1) define the independent interactions between earthworms and two increasingly popular pesticides, 2) introduce the potential of using agar as a medium for earthworm exposure tests, and 3) verify the use of ToxTrac for behavioral analysis in earthworms. This study will contribute to our understanding of the potential exposure effects on an economically important, beneficial non-target species.

**Endothelial Tube Maintenance in a HUVEC cell Model for Myotonic Dystrophy Type 1**

Grace Holcomb
Faculty Advisor: Dr. Ginny Morriss

Myotonic dystrophy type 1 (DM1) is a multi-systemic condition that results in severe muscle weakening and wasting. DM1 is caused by an expanded region of CTG repeats in the 3' untranslated end of the DMPK gene. Muscles require vasculature to supply nutrients and oxygen for muscle maintenance. A previous study involving muscle wasting in a mouse model for DM1, implicated angiogenic genes as contributors to muscle wasting. The ultimate goal of this project is to test whether myokines are involved in communicating between skeletal muscles and vasculature. As a baseline analysis, we wanted to determine whether expression of expanded-CUG repeats in the human umbilical vein endothelial cell (HUVEC) line would disrupt the maintenance of endothelial tubes. The cell line maintenance and passaging were optimized for ideal cell proliferation. HUVEC cells were differentiated, followed by transfection with DMPK exons 11-15 containing either 960 CUG repeats or no CUG repeats, or no additional DNA. Transfected cells were imaged every 3 to 6 hours over 24 hours. Upon visual analysis, the differentiated cells expressing DMPK with a 960 CUG repeat showed degradation of the endothelial tube network when compared to control groups with and without the DMPK gene in both tube-length and tube-width. The quantification of endothelial tube width and length using ImageJ software will establish a baseline response of the endothelial tubes to CUG repeat expression, which can be used to compare further treatments for phenotypic rescue or the effect of conditioned media from myoblast cultures on endothelial tube maintenance and/or development.

**Genomic Similarity to Predict Infection in Bacteriophages**

Kayla Botto
Faculty Advisor: Dr. Lewis

Bacteriophages, also called phages, are viruses that only infect bacteria. Phages are used in phage therapy, which is a new treatment for bacterial infections and hopes to be the solution to antibiotic resistance. Each bacterium has a unique set of phages that can infect it and finding these phages can be difficult and tedious. The aim of this research was to grow phages on *Bacillus thuringiensis kurstaki* (Btk) and do a host range study on an array of *Bacillus* bacteria. Btk was chosen as the host because of its close relationship with *B. anthracis*, the bacterium used to make anthrax. Afterwards the relationship between genomic similarity of the bacteria and phage and probability of a successful infection can be explored to see if it can be used to predict successful infection. Growth of the phages has been a challenge. Different parameters for growth, such as different concentrations of host, different temperatures of growth, and medium additives, have been tested to find the optimal growth environment and process for the phages. Optimization of phage growth will continue into the fall 2021 semester.

**The Role of PGAM5 in Apoptosis in Kinetoplastids**

Hannah Lee
Faculty Advisor: Dr. Swati Agrawal

Kinetoplastids are a group of pathogenic, unicellular parasites that can cause fatal diseases in humans, such as Leishmaniasis and sleeping sickness, most prominent in tropical and developing parts of the world. Although some treatment methods are available for parasitic infections, they are often not optimal and can induce side effects. *Crithidia fasciculata* is a nonpathogenic Kinetoplastid that can be used as a model organism in the lab to study possible treatment methods. A major asset to the parasites' survival is apoptosis which allows for adaptation to the environment as well as avoidance of immune detection by the host. Phosphoglycerate mutase family member 5 (PGAM5) is a metabolic enzyme that has been suspected to play a role in cell death as a pro-apoptotic gene in *C. fasciculata*. This dodecamer protein regulates mitochondrial homeostasis and is associated with the development of diverse diseases. We hypothesize that the absence of PGAM5 will inhibit apoptosis in the parasite, reducing its rate of survival which could possibly create an alternative treatment method for parasitic infections. To replace PGAM5 in the parasite, a gene replacement strategy using the CRISPR-cas9 system followed by homology directed replacement at the PGAM5 locus. We created two drug replacement constructs for neomycin and puromycin resistance using Gibson Assembly. After verifying the sequences by sequencing, the constructs will be transfected into *C. fasciculata*. Once a knockout clone is isolated, knockout parasites will be observed and compared to wild type cells to understand the role of PGAM5 in the apoptosis pathway.

**Apoptosis Induction in Jurkat T Lymphocytes by Proton Pump Inhibitors**

Shreya Murali
Faculty Advisor: Dr. Randall Reif

Programmed cell death, also known as apoptosis, occurs constantly in humans. In healthy cells, proton pump proteins move $H^+$ ions across cell membranes, regulating pH levels inside the cells. Proton pump inhibitors (PPIs), such as omeprazole, prevent the appropriate function of the proton pumps, limiting pH regulation within the cell, potentially causing apoptosis. In previous studies, omeprazole induced death in Jurkat T-lymphocytes; however, there was no confirmation in whether cells died through apoptosis, or necrosis, where the cell lyses. The goal of this research was to use Annexin-V staining to determine if omeprazole induced apoptosis in Jurkat cells. Apoptosis induction was observed by adding Annexin V-FITC and staining cells with propidium iodide (PI) dye. The cells were then imaged using fluorescence microscopy. Apoptotic cells would bind Annexin V-FITC and fluoresce green while necrotic cells would bind PI and fluoresce red. The cells showed apoptosis induction after incubation in omeprazole for six hours and monitored over a 30-hour period. There was a peak at 18.0 hours, with 12.5 ± 2.48% apoptotic cells. In comparison, doxorubicin, a known chemotherapeutic that induces apoptosis, was used as a positive control and peaked at 21.0 hours with 9.55 ± 7.48% apoptotic cells. T-tests were performed between the omeprazole and a negative control, showing that the data was not statistically significant. Future studies will focus on addressing the validity of the staining protocol as well as extending incubation periods.

**Angular Momentum Coherences in Vibrational Molecular Dynamics**

Zoe Rafter
Faculty Advisor: Dr. Varun Makhija

Molecular dynamics describes what happens inside of a molecule (clump of atoms) after some amount of energy is dumped into a system, for instance when light is absorbed by a molecule. In natural systems, this absorbed energy often needs to transfer from one location to another. The vibration of atoms in a molecule is believed to facilitate this transfer. In a particular excited state of the molecule of Nitrogen Dioxide ($NO_2$), the bending and stretching of bonds is known to transfer energy from one vibrational state to another. This energy transfer is called Fermi Resonance. One potential way to image this vibration of a molecule is using ultrashort laser pulses. Ultrashort laser pulses last approximately a millionth of a billionth of a second, and act as a very short "flash" of a camera, during which the vibrations of the molecule are frozen. Such an experiment was recently attempted; however, the molecules were arbitrarily oriented and angular momentum was not considered. This arbitrary orientation effectively "blurs" the image. To remove this "blur", a calculation of the excitation step, including angular momentum must be carried out. Therefore, we include the angular momentum states of $NO_2$ and computationally simulate the vibrational motion including angular momentum in the excited state.

**Bootstrapping Training Data for a Political Polarization Classifier**

Alexis Kochanski
Faculty Advisor: Dr. Stephen Davies

Polarization in the political sphere, seen through combative communication and stalemate, may impose negative social impacts on the population. Attempting to measure political polarization in the masses through self-reported surveys and interviews can present response biases of social desirability. The classification of thought freely written online allows for political polarization to be measured in an impartial manner. Our research aims to measure the degree of political polarization over time by collecting and classifying threads of dialogue within political communities on the anonymous forum website Reddit.

Our team utilized Reddit APIs to gather threads of text from multiple communities of subreddits from the internet. As a team of four, we initially hand-annotated a small subset of threads and evaluated our individual labels of "polarized" or "nonpolarized" for unanimity. To produce a larger training set of labeled data out of our unlabeled data, we employed the method of bootstrapping data, which is known to improve a classifier's accuracy. Prior labeled training data is used to train a classifier that will then classify a set of unlabeled data. The data points with the highest probability of being accurately labeled with their designated class then become a part of a new set of training data. The classifier is reconstructed with the new set and the process is repeated until an iteration through the bootstrap classifier results in an average accuracy less than the previous iteration. Preliminary efforts to bootstrap data have begun to show improvements in our political polarization classifier's accuracy.

**The Effects of Coal Ash Concentration on the Development, Hatching Rate, and Reproduction in *Planorbella duryi***

Catherine Crowell
Faculty Advisor: Dr. Frankel

Coal ash (CA) is an industrial waste that is produced by coal-burning power stations which contains various trace metals. While numerous studies have examined the effects of large coal ash spills on aquatic vertebrate species, little is known on the effects of CA leachates (CALs) on aquatic invertebrates. The goals of this study were to assess the impact of CALs on 1) the development of embryonic *Planorbella duryi*, 2) the hatching rate of embryonic *P. duryi*, and 3) the reproduction of adult *P. duryi*. To create CALs, 0g to 50g of CA was added to glass vessels containing pH-adjusted synthetic water which were then vacuum filtered and analyzed for trace metals using ICP-OES. Embryonic *P. duryi* clusters (<24hph) were exposed to each leachate for 10d and images were obtained every 24hrs to assess viability and development stage. For the reproductive assay, two adult *P. duryi* were placed into a glass vessel and exposed to a specific leachate treatment level for 9d. Newly-laid clutches were quantified every 24hrs. Preliminary results indicate individuals exposed to the higher treatments laid fewer egg clutches and exhibited delayed embryonic development. This study will provide essential information on the effects of CALs on multiple sublethal endpoints with implications for multiple trophic-level interactions within aquatic ecosystems.

**Rotational Dynamics of Asymmetric Molecules**

Madeline Killian
Faculty Advisor: Dr. Varun Makhija

In nature, light is constantly interacting with molecules. Understanding these interactions gives us more insight into what our world is made up of. When light hits a molecule, it is absorbed by the electrons in the molecule. The overarching research goal is to make a movie of the electrons after light hits the molecule by using a femtosecond (a millionth of a billionth of a second) laser pulse. A molecule's natural rotation creates a blur in this movie. The goal of this research is to understand the rotation of the asymmetric chloroethylene ($C_2H_3Cl$) molecule in order to get rid of the blur it creates in the electron movie. Similar research has been previously conducted for the symmetric molecule ethylene ($C_2H_4$). The asymmetry of $C_2H_3Cl$ results in complicated probability distributions for rotational orientation after a laser pulse hits the molecule. We determine these probability distributions computationally for $C_2H_4$ and $C_2H_3Cl$. The results show that for $C_2H_3Cl$ there is a highly asymmetric distribution of probabilities and a unidirectional rotation; this is not observed in $C_2H_4$. This is the first step towards being able to image electronic motion in $C_2H_3Cl$.

**Understanding the Role of the Bax-1 Inhibitor and AATF Genes in Apoptosis of Kinetoplastid Parasites**

Abigail Delapenha
Faculty Advisor: Dr. Swati Agrawal

Leishmaniasis is prevalent in developing countries, infecting 1.5 to 2 million people per year. Drugs used to treat Leishmaniasis can quickly develop resistance and have strong side effects, such as Paromomycin which causes ear poisoning and Amphotericin which can cause nephrotoxicity. Crithidia fasciculata is a useful model organism for studying Leishmania, a pathogenic trypanosomatid parasite. Apoptosis in kintetoplastid parasites is suspected to allow the parasites to escape immune detection and select for the fittest parasites for host infection. Understanding the apoptosis pathway in C. fasciculata can be used to develop alternative drugs. We are studying two genes, Bax-1 inhibitor and AATF that have been characterized as anti-apoptotic genes in higher eukaryotic organisms. Knock out mutants of these genes will be created using CRISPR-Cas9 technique, to replace the gene locus with a drug resistance cassette. Polymerase Chain Reaction (PCR) was used to amplify three fragments of DNA (5' UTR, 3'UTR, and drug cassette). The 500bp UTRs allow for recombination of the construct and the drug cassette allows for selection of successful knock out parasites. These fragments were fused together using fusion PCR. The bax-1 puromycin, AATF neomycin, and AATF puromycin constructs have been verified and transfected into the DNA of Crithidia. PCR to confirm the integration in the genome of C. fasciculata is in process. If the genes are successfully knocked out, the rates of apoptosis in the wild-type and knock out parasites will be compared to determine the role of the Bax-1 inhibitor and AATF genes in apoptosis.

**Assessing the Impacts of the Common Deicing Agent NaCl on the Viability, Embryonic Development, and Behavior of the Freshwater Snail *Physa acuta***

Sophia Weldi
Faculty Advisor: Dr. Tyler Frankel

Nearly 24.5 million tons of road salts are distributed annually on roadways in the United States. Up to 90% of these applications utilize NaCl, of which 55% has been shown to directly enter freshwater ecosystems via runoff. While the USEPA recommends that NaCl concentrations do not exceed a four-day average of 230mg/L more than once every 3 years, recent studies have observed concentrations of over 600mg/L. NaCl has been found to inhibit algal growth, reduce respiration rates of bacteria in activated sludge, and increase mortality in all life stages of some amphibians. However, the effects of NaCl on aquatic invertebrates has been relatively unexplored. Thus, this study assessed the effects of NaCl exposure on 1) *Physa acuta* egg cluster viability and development and 2) locomotor and egg deposition behaviors. Egg clusters (<24hph) were collected and exposed to 0, 100, 250, or 500mg/L NaCl for 10 d using a static exposure method. Viability and developmental stage of each embryo was quantified every 24hrs. Mobility was recorded and quantified on days 0, 3, and 7 using ToxTrac (v. 2.83). Preliminary results indicate that adults exposed to 1000mg/L exhibit decreased average mobile speed, total distance travelled, and egg clutch deposition with more eggs deposited per clutch. Embryos exposed to 500mg/L exhibited decreased hatching success. These findings provide novel insight into the impacts of a commonly utilized deicing agent on a non-model freshwater invertebrate species, suggesting that similar effects may also be exerted on endangered or keystone aquatic invertebrate species.

**Using Machine Learning to Identify Political Polarization on Social Media**

Veronica Cagle
Faculty Advisor: Dr. Stephen Davies

There has recently been an increase in political conversation on social media platforms. Reddit is one social media application that allows users to anonymously share their opinions and discuss political topics; this text can be used to measure the political climate at any given time. We gathered two decades worth of political content from Reddit to investigate whether there was a change in the degree of political polarization over time.

We created a machine learning classifier that can predict whether a thread posted on Reddit is polarized or not. Polarization is a nuanced concept that manifests itself in a variety of ways. We defined polarized discourse as that which is combative, argumentative, stubborn, and extreme in viewpoint. We used a multi-layer feed-forward neural network which we trained on data that our team hand-tagged as polarized or not polarized. A neural network takes the data as input and goes through a series of layers to search for patterns in the text. The neural network predicts whether a new text, that it has not been trained on, is polarized or not. We experimented with features such as word embeddings, stemming, lexical diversity, removal of stop words, and bigrams to improve the accuracy. We achieved the highest accuracy with the combination of stemming, measuring lexical diversity, and using bigrams.

**Temporal Dynamics of the Intrinsic Pathway of Apoptosis via Doxorubicin Induction**

Ramsey Cotton
Faculty Advisor: Dr. Randall Reif

Apoptosis, or programmed cell death, is a regulatory process which occurs to keep a constant cell count within the body. The misregulation of this process can lead to tumor growth. There are multiple pathways in which apoptosis may be induced, through external stimuli at the cell membrane receptors or internal DNA damage, which triggers caspase enzymes that cleave proteins in the cell. The intrinsic pathway is the focus of this study. The timing of caspase activity during the apoptotic process is not well known. This study was conducted in order to understand the timing of caspase activity for caspase-targeted drug therapies. Doxorubicin, a chemotherapy drug capable of inducing apoptosis through the intrinsic pathway, was studied in Jurkat-T Lymphocytes captured on a microfluidic device. Caspase activity was monitored using fluorescence microscopy with L-asparticacid-Rhodamine110($D_2R$), a fluorescent probe capable of tracking general caspase activity in cells. The cells were monitored over a period of 9 hours. Preliminary data showed that for overall caspase activity, the onset time most commonly occurred around 6.3 hours, with an average duration of 180 minutes. This suggests that caspase activity continues past the 9 hour time trial. Once additional data is acquired, a longer study may be required to observe the entire period of general caspase activity.

**Effect of Social Hierarchies on Exercise in Social Mice**

Rachel Myrick
Faculty Advisor: Dr. Parrish Waters

Mice are social animals that form hierarchies in which dominant animals control limited resources. Mice will perform work to gain access to a running wheel, demonstrating the rewarding nature of this stimulus. We established four social cages of three mice, and limited access to a running wheel using gates that recognized each mouse through RFID technology. Using these methods, we can determine individual wheel running activity of mice living in social groups. We expect dominant mice to control the running wheel and enter the gates more often than subordinate mice. We used the tube test, sociability test, and recorded home cage behavior to determine social rank, and assessed anxiety-like behavior, cognition, and stress hormones to explore other qualities that may be associated with dominance rank. As a control group, we individually housed 6 other mice with running wheels to determine typical patterns of wheel running and performed the same analyses on these mice. Our analysis of results is forthcoming.

**Morphological Changes in Non-Native Fish Species Influenced by Differences in Upstream and Downstream Habitats**

Alexander Fernandez
Faculty Advisor: Dr. Lamphere

When species are introduced to a new area, they are often subjugated to many different selection pressures that may affect the body shape of the introduced species. The purpose of this project is to measure change in body morphology for a species of minnows, *Campostoma anomalum*, recently introduced to the Rappahannock drainage and to see if body shape was correlated to upstream and downstream habitat. Upstream habitat typically is considered to be rocky, complex habitat with high flow that is believed to select for fish that have a more steady swimmer body shape while downstream habitat offers slower waters with simpler habitats that are better suited for an unsteady swimmer body shape. To do this, *Campostoma anomalum* were sampled from 12 sites in the Rappahannock drainage and separated into upstream and downstream sites based on location on the Rappahannock and Rapidan Rivers. Once collected, the fish were photographed, landmarked, and underwent a principal component analysis (PCA) through thin-plate spines (TPS). Through the PCA, it was found that individuals with a low PC1 had smaller eyes and body length and those with a low PC2 had deeper bodies. Additionally, upstream sites tended closer to a lower PC1 than downstream sites. However, a linear trend between distance from the most downstream site and either PC was not observed, likely due to differences between the microhabitats playing a large role in affecting *Campostoma anomalum* body shape than originally expected.

**Myokine Expression in a Myotonic Dystrophy Type 1 Cell Culture Model**

Abigail Vorsteg
Faculty Advisor: Mr. Morriss

Skeletal muscle wasting is the predominant cause of myotonic dystrophy type 1 (DM1) related mortality, though the specific mechanism responsible for muscle wasting in DM1 individuals remains undefined. DM1 is an inherited muscular disorder caused by expanded CTG repeats in 3' untranslated region of DMPK gene that results in toxic gain of function of the transcribed mRNA produced by the gene. Myokines are proteins secreted by skeletal muscles that are involved in cell-cell communication and have been linked to DM1. The objective of this research was to explore how DM1 alters the expression of and the relationship between the myokines in skeletal muscle cells. Mouse myoblast (C2C12) cell lines were cultured and then transfected with DNA plasmids containing the final four exons of the human DMPK gene containing either 0 or 960 CTG repeats to represent DM1 in skeletal muscle cells, or the cells were mock-transfected. Myoblasts were then differentiated into myotubes, and RNA was extracted from both undifferentiated and differentiated cells at three time-points. cDNA was generated from the isolated RNA and will be used to quantify the relative expression levels of specific myokines in myoblasts and myotubes via qPCR. Future aims of this research include the study of specific myokines' roles in skeletal muscle wasting mechanisms in DM1.

**Synthesis of Indazole Inhibitors of KasA, a Vital Enzyme of *M. tuberculosis***

Karissa Highlander
Faculty Advisor: Dr. Oldham

Tuberculosis is a disease that affects the lungs caused from Mycobacterium *tuberculosis* and is the leading cause of death by infectious disease in the world. Although drug treatment options exist, in recent years increased rates of antibiotic resistant strains have become more prevalent driving a need for new treatment approaches. KasA, a β-ketoacyl synthase, has been found to synthesize parts of the cell wall and been identified as an attractive drug target. An effective competitive inhibitor of KasA would block the enzyme from binding the substrate, preventing elongation of the backbone and creation of the mycolic fatty acids that form the mycobacterial cell wall, ultimately killing the bacterium. An inhibitor of KasA known as DG167 was used as a scaffold model of tuberculosis for this research. To begin, 6-nitroindazole underwent an alkylation reaction, which methylated a nitrogen, resulting in a mixture of products from which the major product was produced in 49% yield. Once the 1-methyl-6-nitroindazole was purified, it was reduced using iron powder converting the original nitro group into an amino group in 85% yield. After the 1-methyl-6-indazolamine was formed, various derivatives were synthesized including both sulfonamides and amines. There was a range between 36% and 84% yield amongst all derivates. AutoDock Tools, an automated docking computer program, was used to test the interactions between inhibitor and each derivative in order to predict suitability of the drug candidate. For future research, the derivatives will be tested *in vitro* to determine their effectiveness as potential drugs.

**Using Additive Manufacturing To Increase Reproducibility In A Packed Bed Column**

Docia Atanda
Faculty Advisor: Dr. Sarah Smith

Additive manufacturing (3D printing) is a transformative approach to industrial production that uses computer aided design (CAD) software to direct hardware to deposit material layer upon layer to deposit material in precise geometric shapes to yield lighter, more complex, and low-cost designs with increased reproducibility. One area where 3D printing can improve current methods is packed bed columns. Packed bed columns are used in many chemistry processes such as separations, distillation, catalysis, and water treatment. Typically, columns are slurry packed with a granular material and have bed inhomogeneity, low reproducibility, and do not provide optimal mixing and contact between the stationary phase and mobile phase due to channeling and path preference by the mobile phase. By 3D printing columns with specific internal geometries and channels, the reproducibility and homogeneity can be improved. In this research, multiple columns were designed with controlled paths to control packing, particle size and shape to enable conditions optimal for the removal of highly charged metals that are hazardous to the environment in water samples by iron oxide or carbon. The columns and caps were designed in Fusion 360, sliced through the Dremel DigiLab 3D Slicer, and printed with the Dremel DigiLab 3D40 Idea Builder printer using polylactic acid (PLA) filaments. The printed columns were each connected to a pump, and it was determined that none leaked at a flow rate of 1 mL/min.

**Paleoclimate analysis using growth bands and stable isotopes from mid-to-late 1700s Stratford Hall oysters**

Lyra Winters
Advisor: Dr. Pamela Grothe

High-resolution paleoclimate studies from fossil oysters, *Crassostrea Virginica,* have the potential to provide seasonal climate variability records and inform how climate may have contributed to major historical events. Stratford Hall plantation in Westmoreland County, VA, for example, prospered economically until the last 1700's when many of its slave quarters were backfilled. The objective of this research was to determine if multidecadal climate change near the end of the Little Ice Age could have played a role in the demise of the Stratford Hall plantation. Previous work established that *Crassostrea virginica* precipitates its shell in isotopic equilibrium with the water, making it an excellent recorded for seasonal variability. We developed SEM oyster growth band- $\delta^{18}O$ models for six fossil oysters collected from the infilled slave quarters at Stratford Hall which were $^{14}C$ dated to ~1756 to ~1779 CE. We found that the older shells had a smaller range in $\delta^{18}O$ (~-2.8% to ~-7.3%) and smaller growth averages during both the winter and summer seasons (~-0.84 and ~-1.3 mm/season; respectively). The youngest shell range of $\delta^{18}O$ was -2.8% to -7.3% and exhibited the largest growth during both warm and cold seasons (1.74 and 1.12 mm/season; respectively). These results suggest a change from a colder, harsher climate to a warmer climate with more seasonal variability. Our results are in agreement with previous studies that show an increase in seasonality on multidecadal timescales in this region. We suggest that prolonged cold and harsh climate conditions during the mid-1700's may have played a role in the economic decline of Stratford Hall plantation.

**A Numerical Study of COVID-19 using the SVIR Model**

Caitlin Holt
Faculty Advisor: Dr. Lee

This research project consisted of using numerical methods to investigate trends in infections and vaccinations for severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), which will be referred to as COVID-19, using four ordinary differential equations. The first doses of the COVID-19 vaccine were administered in December 2020, and the number of people becoming fully vaccinated is rapidly increasing. Graphs generated from the model could predict future trends in infection and vaccination rates, which can provide time for appropriate actions to be taken to avoid possible major outbreaks. MATLAB codes were developed to approximate the solution to the model using algorithms derived from numerical methods such as Taylors, Runge-Kutta, and multi-step methods. Data, such as infected and vaccinated populations, were collected from the start of the vaccinations in December 2020 to July 2021 from various sources, including the CDC. These data were used to estimate parameters when using the model to graph the COVID-19 trends in the United States. The resulting graphs from the model are not as accurate as desired, specifically the equation for the infected population consistently overestimated trends when compared with actual data.
However, as the vaccinated population increased, the infected population began to significantly decrease, demonstrating positive effects of the vaccine.