Summer Science Institute Research Symposium 2013

Wednesday, July 24th
Jepson Science Center, Room 100
University of Mary Washington

Summer Science Institute
2013 Symposium

Schedule of Events

MORNING ORAL PRESENTATIONS ..... 9:30 – 11:20

9:30……..ERIC JOHNSON
9:50……..KYLE GENOVESE
10:10 ……BRYAN FINCH

10:30 – 10:40 ..... BREAK

10:40…… KATHIE BELROSE-RAMEY
11:00……..CASEY HOWREN

MORNING POSTER SESSION ..... 11:20 – 12:30

MICHAEL CRAWFORD, NGOC QUYEN HUYNH, DANE LAWHORNE,
CARTER MOORE, JENNA STOCKTON, YOSHI TAKEDA

LUNCH..... 12:30 – 1:10

AFTERNOON ORAL PRESENTATIONS ..... 1:10 – 2:30

1:10…….DALTON ECHARD
1:30……PATRICK MULLEN
1:50 ……...CHIARA TORNABENE
2:10……...TERESA FENN

AFTERNOON POSTER SESSION ..... 2:30 – 3:40

BROOKE ANDREWS, SAMUEL ARUTYUNYAN, KIMBERLY HILDEBRAND,
KATELYN JONES, PHILIP WAHLMAN

AWARDS CEREMONY 4:00

Oral Presentations

Conversion of Hydroxyl Functional Groups to Azido Functional Groups for Use in Click Chemistry

Eric Johnson
Faculty Advisor: Dr. K. Nicole Crowder

Since the discovery of copper-catalyzed azide-alkyne cycloaddition click reactions, the ability to convert a terminal functional group into either an azide or alkyne has become a valuable asset. Some functional groups, such as hydroxyl groups, are more difficult to replace than others due to the fact that they are poor leaving groups. In order to convert a terminal hydroxyl group into an azido group, two step reactions are used where an intermediate is generated with an easily replaceable leaving group; the intermediate then undergoes a reaction to yield the desired azido functional group. In this research, 1-heptanol and 11-hydroxyundecylphosphonate bound to a copper surface, compounds containing a terminal hydroxyl group, were reacted with either phosphorus tribromide (PBr_3) or methanesulfonyl chloride (MsCl) to generate these intermediates. The PBr_3 generated a bromide intermediate, while the MsCl generated a mesyl intermediate. The resulting intermediate was then either reacted solely with sodium azide to generate the azido functional group or used in an in-situ click reaction to generate a triazole. Analysis performed using infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy indicated that the reactions need to be optimized.

Modeling Economic Growth in Developing Countries

Kyle Genovese
Faculty Advisor: Dr. Julius Esunge

Isolating key factors that contribute to economic growth could ultimately lead to improving economic conditions for developing nations. For this problem we use multiple regression to predict the Gross Domestic Product (GDP) of African countries. Three models are constructed: first, the Common Market for Eastern and Southern Africa (COMESA) economic region, second, a smaller economically-related group of countries within COMESA, and third exclusively for Ethiopia. Each model provides information about indicators that affect each set of GDP's. The results are a significant step towards revealing the keys to economic growth in developing countries.

Using Camera Trapping to Monitor Wildlife in Stafford County, Virginia

Bryan Finch
Faculty Advisor: Dr. Wieland

Camera trapping as a method for population census is relatively new in wildlife biology, however, it is quickly increasing in popularity as researchers come to realize its benefits. In general, camera trapping consists of using a number of cameras equipped with motion detectors placed in a given area to "capture" photographs of wildlife. These pictures can then be employed to derive information on everything from animal behavior to abundance. This project employed the use of trail cameras on the University of Mary Washington Foundation's property to gain knowledge about the wildlife and about camera trapping as a sampling tool. The University of Mary Washington Foundation's Stafford-West property is a parcel of about 260 acres, located in Stafford County just a few miles northwest of the UMW Stafford Campus. This property was acquired by the Foundation in December of 2008. A variety of wildlife has been reported as occurring in the area but no documentation is available for the majority of these. Eighteen trail cameras were placed in a series of 500 m2 quadrants throughout the property to continuously gather photographs for 35 days. Photographs were examined to identify species, and analyzed to obtain information on relative abundance, activity patterns, and frequency of detection. Fourteen different species of birds and mammals were photographed including black bear, white-tailed deer, coyotes, and wild turkeys. The Relative Abundance Index (RAI) for both white-tailed deer and grey squirrel were the highest at 1.8, followed by opossum (RAI= 0.52), raccoon (RAI= 0.47), coyote (RAI=0.29), black bear (RAI=0.17), and wild turkey (RAI=0.12). We plan to continue monitoring throughout the fall and winter to obtain a more complete data set.

Locating the Binding Site of RAI1 within the CLOCK Regulatory Region

Kathie Belrose-Ramey
Faculty Advisor: Dr. Deborah Zies

Smith-Magenis Syndrome (SMS) is a neurobehavioral disorder characterized by mental retardation, sleep disturbances, obesity, and behavioral disorders. SMS is caused by haploinsufficiency of the retinoic acid-induced 1 (RAI1) gene, which is a transcription factor involved in the regulation of many genes. Previously, a Chromatin Immunoprecipitation-microarray chip (ChIP-chip) experiment was conducted to determine genes regulated by RAI1. The gene chosen for this study was Circadian Locomotor Output Cycles Kaput (CLOCK). The overall goal of the study is to identify the RAI1 binding site. To that end, the region of CLOCK identified by ChIP-chip was used to create a pGL3 luciferase reporter gene construct. Luciferase assay testing of the original construct and a series of deletions narrowed the RAI1 binding site to a 50 bp region. Concerns about possible false positive results with the pGL3 reporter system led to the decision to move the CLOCK regulatory region to the updated pGL4 system. The specific goals of our summer research have been to create some constructs similar to the pGL3 constructs in the improved pGL4 system and to implement a new deletion strategy to the pGL4-CLOCK construct. Three constructs similar to those in pGL3 are completed and two new deletion constructs are being confirmed by sequencing. Next, luciferase assay testing will be conducted to both determine if the pGL4 constructs give similar results to the pGL3 constructs and to continue to narrow down the RAI1 binding site within the new constructs. Identification of the RAI1 binding site would enable researchers to identify other genes regulated by RAI1 and could lead to new treatments for Smith-Magenis Syndrome and other conditions related to RAI1 gene expression.

A Numerical Analysis of the S I R Model for Modeling Epidemics

Casey Howren
Faculty Advisor: Dr. Leo Lee

In this research project, we use numerical approximation techniques to model the projected course and severity of epidemics, while focusing specifically on the 2009 H1N1 flu pandemic. Our model is based off of the commonly used S-I-R model for epidemics, which models the relationships between the Susceptible, Infected, and Removed classes of a population that a disease is affecting. An exact solution is derived for the model using elementary algebra and calculus techniques. An algorithm is then developed using the numerical approximation method of Euler's Method and a corresponding MATLAB code is created to compute numerical solutions and plots that give an approximated model of an epidemic. The built-in MATLAB function ode45 is used to compare the results of our program to computer-generated results, which ensures accuracy. Our methods are then applied to real world data in order to model the behavior of the 2009 H1N1 pandemic in the United States. After applying the numerical methods to real world data, we created hypothetical epidemic situations to demonstrate the applicability of our model. This work seeks to show that using mathematical methods to model epidemics can accurately predict the behavior and severity of a disease in a manner that is more efficient and less complicated than methods for exact solutions, which can then allow for the creation of efficient prevention and treatment plans that will in turn ensure that an epidemic has the least impact possible on a population.

RESPONSIVITY OF SOLAR CELLS AND PHOTO DIODES

Dalton Echard
Faculty Advisor: Chinthaka Liyanage

Photovoltaic cells are a commonly used as a source of renewable energy, and should be optimized for peak efficiency. In order to optimize a solar cell it is important to know the spectral sensitivity of the device, that is, what wavelength of light the photovoltaic cell produces the most current. This experiment was conducted by using the calibrated lamp as a light source that was guided through a monochromator. The spectral range of the monochromator was 350nm to 1100nm. This light was then sent through an optical chopper, the light was then incident onto a photovoltaic cell. The photocurrent of the cell was measured using a lock-in-amplifier. A responsivity curves were created for each of the devices, a research grade calibrated photo diode and a commercially available solar cell. The photo diode revealed a peak current around 970 nm. The commercial solar cell had a peak current at 590 nm.

Absorption Spectroscopy of Rubidium

Patrick Mullen
Faculty Advisor: Dr. Hai Nguyen

This project focused on the creation and implementation of an advanced optical system to perform saturated absorption spectroscopy of rubidium vapor. Laser absorption spectrometry is a popular method used to analyze elemental vapors for any number of properties. These properties include refractive index, quantum hyperfine structures, and contamination coefficients. In order to produce such an experiment we had to create and verify a Radio Frequency modulated, temperature controlled diode laser of a 795nm wavelength. This laser was used as a source for an optical system in which the beam was focused and passed through a rubidium cell where it would then reach a dual photo diode detector. Using this optical setup we were able to analyze the hyperfine structure of rubidium and show its controlled fluorescence. The hyperfine structure known as the D1 transition is established and verified to the extent that our equipment would allow.

Biostratigraphic Significance of the Ostracodes from the Dinosaur Bearing Cedar Mountain Formation

Chiara Tornabene
Faculty Advisor: Dr. Neil E. Tibert

Ostracodes are bivalved crustaceans that live in marine and nonmarine waters. Given their long fossil record, they provide the earth scientist a tool to determine both age and environment. The genus *Cypridea* is a well known nonmarine lineage reported from the early Cretaceous Purbeck/Wealden deposits of England and Germany that serves as an important biostratigraphic indicators.

The Cedar Mountain Formation in central Utah contains an exceptional vertebrate faunae that records the radiation of Lower Cretaceous dinosaurs of global significance. The age of the Cedar Mountain Formation is assigned to the Barremian-Aptian (125-120 Myr) on the basis of *Utahraptor ostrommaysorum*, pollen, and charophytes (green algae). Reports of the ostracode *Cypridea setina* from a single locality in the Yellow Cat Member of the Cedar Mountain Formation in central Utah indicate that the deposit is potentially Berriasian-to early Valanginian in age (145-140 million years old). Our goal is to characterize the ostracodes in sufficient detail to better constrain the age of this important dinosaur bearing formation.

We evaluated a suite of samples from two Cedar Mountain sites that includes Lake Madsen Site (Yellow Cat Member) and Scott's Ostracode Site (Poison Strip Sandstone). The rich ostracode association includes *Cypridea setina*, *Candona* sp., *Alicenula* sp., and *Cypris* (?). Our results indicate that the fauna is much more diverse than originally reported and therefore the age of the deposit remains in question. Further taxonomic work on the ostracodes will provide insight on the age of the Cedar Mountain Formation.

Impact of Acid Mine Drainage on Soil Phosphorus, Metal Content, and pH in a Riparian Environment

Teresa Fenn
Faculty Advisor: Dr. Melanie Szulczewski

We are studying the soil profile of Contrary Creek in Louisa County, Virginia, to better understand how acid mine drainage (AMD) is affecting the ecosystem. AMD can lower the pH of the surrounding soil which increases the solubility of the metals that are present, which may be harmful to the environment. Organic phosphorus may affect the availability and distribution of metals in the soil by binding with the surfaces of metal bearing minerals. The effects can vary with depth. Composite soil samples were collected at three depths at five sites along the stream with the central site at the abandoned mine. The soil samples were digested with nitric acid and hydrogen peroxide according to EPA Method 3050B and analyzed with an inductively coupled plasma-atomic emission spectrometer (ICP-AES) to determine the concentration of lead, iron, aluminum, arsenic, and other metals. Total soil organic phosphorus was measured by the ignition method. Soil pH decreased with depth and was lowest at the mine site. Total organic phosphorus ranged from below the detection limit to over 400 mg kg-1. It was strongly positively correlated with some metals, while negatively correlated with others. Lead and arsenic concentrations were highest at the mine site in all layers of the soil, while iron was highest at the mine site in the lowest layer. Aluminum concentrations were highest upstream of the mine site in all soil layers. Further studies will be conducted to better understand how and where the products of AMD interact with the environment.

Poster Presentations

Estimating the effects of heterogeneous competition in an agent-based ecological model using GIS raster color

Michael Crawford
Faculty Advisor: Dr. Stephen Davies

It is hypothesized that inter-species competition is one of the main factors that determine the range and distribution of Sensitive joint-vetch, a rare, tidal wetlands annual. The precise effects of this competition, however, are poorly understood by ecologists and difficult to quantify. This is often the case in the field of modeling and simulation, and requires researchers to make an informed guess about the subject of their study and approximate the effects as best they can.

We have constructed a detailed, individual-based simulation of Sensitive joint-vetch in its Holts Creek, Virginia, habitat. Although the life-history transitions of the plant have been identified and quantified, and experiments have been performed to isolate competition on a small, m2 plot scale, little is known about the aggregate effects of competition. In order to elucidate these landscape-scale effects, we propose a new method of distinguishing poor from high quality plots that uses GIS to correlate the pixel color of an individual plot to its propensity for sustaining joint-vetch. This propensity is then used to determine the vital rates of a given plot and is applied to all plants within it. Results indicate that inter-species competition plays a limiting, though by no means exclusively important, role in the spatial arrangement and rarity of joint-vetch. Based on the spatial patterns that joint-vetch exhibits in silico, it appears that other environmental factors such as ground saturation and distance from the stream must also play a crucial role.

Fabry-Perot Interferometer

Ngoc Quyen Huynh
Faculty Advisor: Dr. Hai Nguyen

This summer we were able to set up a Fabry-Perot Interferometer Spectrum Analyzer (FPA). By setting up a FPA, it is possible to measure and control the spectral structure of the frequency of a laser beam. The Fabry-Perot Interferometer transmits the laser beam through two confocal reflecting mirrors cavity, called the etalon, that tunes the wavelength, and then through a photodiode. The photodiode from the FPA is connected to an oscilloscope displaying the signal data from the beam including the interference of constructive and destructive waves, which results in higher or lower resolution also known as finesse. Using this FPA, it is possible to control and scan the frequency of a laser to a certain single-frequency, so for any future research involving lasers, we could get higher resolution spectroscopic results. Further details on the setup and applications of the Fabry-Perot are shown here.

Analogies Between the Real and Digital Lines and Circles

Dane Lawhorne
Advisor: Dr. Randall Helmstutler

Digital topology is the subfield of topology concerned with the topological properties of digital images. Two basic objects of study are the topological spaces known as the digital line and the digital circle. Although these spaces have roots in digital image processing, we study them from a pure mathematics viewpoint. In many ways, the digital line and digital circle can be viewed as discrete versions of the real line and unit circle. We show that several well-known results about the real line and unit circle have analogs in the digital line and digital circle. For example, it is well-known the real line has a trivial fundamental group, is a covering space of the unit circle, and has an isometry group consisting solely of translations and reflections. It is also well-established that the fundamental group of unit circle is isomorphic to the integers under addition. Our research verifies digital versions for each of these results. We prove that 1) the digital line has trivial fundamental group, 2) the digital line is a covering space of the digital circle, 3) the digital circle has a fundamental group isomorphic to the integers under addition, and 4) the automorphism group of the digital line consists solely of translations and reflections.

A Fossil's Tail: The Environmental Evolution of the Carboniferous from Aquatic to Terrestrial Environments

Carter Moore
Faculty Advisor: Dr. Neil E. Tibert

Nova Scotia contains some of the most complete exposures of Carboniferous sedimentary rocks on planet earth. Some of the earliest pioneers of geology studied the vast formations of the province (e.g. Sir Charles Lyell and Sir William Dawson). These sedimentary rocks record the transition from marine to terrestrial ecosystems. The deposits include the Mississippian Horton Bluff Formation, known for the earliest tetrapods, and the Pennsylvanian coal measures of the Joggins Formation that contain exceptional fossil assemblages of plants, insects and early reptiles. Although the paleobiological significance of these deposits is well established, the environment of deposition still remains very controversial in the context of marine versus non-marine deposition.

Ostracodes are bivalve crustaceans that live in aquatic environments ranging from freshwater to marine. They have a long fossil record with known distributions in carboniferous sedimentary deposits in Nova Scotia. Analysis of shale samples collected from the Horton Bluff formation as well as Joggins, Boss Point, and Port Hood Formations reveal an ostracode association that includes: 1) *Velatamorpha altilis* with non-marine/brackish affinities; 2) *Gutschicka* sp. with similar non-marine/brackish affinities; and 3) *Bairdia* new species with well-known marine affinities elsewhere in Atlantic Canada.

During our field investigations this past summer, a new discovery from the Mississippian Horton Bluff Formation revealed a trilobite with unequivocal marine affiliations. The trilobite indicates the earliest fossil forest and ecosystem had a significant marine influence with shelf like conditions. In contrast, the Pennsylvanian samples, collected from the Joggins Boss Point and Port Hood Formations, confirms that the system was predominately brackish with minor marine influence. Together, these finding highlight the significance of Carboniferous deposits in Nova Scotia that records an elegant pattern of marine transgression and regression that contributed to the evolution of the earliest non-marine faunas.

Fractionation of Metal Contaminants with Soil Depth in an Acid Mine Drainage-Impacted Ecosystem

Jenna Stockton
Faculty Advisor: Dr. Szulczewski

Acid mine drainage (AMD), a result of anthropogenic activity due to resource extraction, continues to harm an ecosystem long after mining operations have ceased. Contrary Creek is an 8-km stream located in Louisa County, Virginia, and the site of a few abandoned pyrite mines that closed almost a century ago. The surrounding ecosystem is still exhibiting strong signs of AMD impacts as a result of the mining operations and remaining tailings. Soil samples were collected from sites upstream and downstream of an abandoned mine shaft about 5 m away from the creek. Soil samples were collected at 0-10cm, 10-20cm, and 20-30cm to determine the availability of metals with depth. The samples were analyzed for trace metal concentrations, pH, and other factors. The soil samples were digested with acid and hydrogen peroxide to determine total metal content. A sequential extraction was also performed on the soil samples to differentiate the distribution of metals within the soil. Although the pyrite mines closed in the 1920s, pH values in the water and soil remain very low. The pH values show a significant decrease between the top layer and the subsoil at most sites. The trace metals Al, Fe, As, Cu, and Pb were of primary focus and were found at concentrations that are detrimental to the creek ecosystem. Studies will continue to analyze the impact that AMD has had on this damaged ecosystem.

Turtles of the Fredericksburg Canal: Estimates of Population Sizes and Growth Rates

Yoshi Takeda
Faculty Advisor: Dr. Werner Wieland

This is an ongoing study entering its second year on turtles living in the Fredericksburg Canal. The objectives for summer 2013 were to confirm the species of turtles living in the canal based on 2012 collection and obtain life history information, including estimating population size. Hoop nets were placed along a 150 m stretch of the canal in the general area as last year and checked daily. All turtles captured were examined for identifying marks from the previous year and new (unmarked) turtles were given individual marks. Length of carapace and plastron and body weight was recorded for each individual and we attempted age determination by counting the number of ridges on the plastron. Population size was determined by open population mark-recapture models using the computer program, MARK (USGS Patuxent Wildlife Research Center software archive). Turtles captured this year: red-bellied cooters (*Pseudemys rubriventris*), painted turtles (*Chrysemys picta*), common snapping turtles (*Chelydra serpentina*), and red-eared sliders (*Trachemys scripta elegans*). Estimates include population size and 95% confidence interval: red-bellied cooters, 36 (26-69); painted turtles, 22 (20-35); red-eared slider, 25 (19-112), common snapping turtles 8 (8-8). Satisfactory growth rates could not be extrapolated for several reasons. Growth ridges on many proved interpreting difficult. Also, there were few recaptures from the previous year. However, plastron length versus weight relationships were found for red-bellied cooters and painted turtles. As is the case with studies of wild populations, obtaining sufficient data to draw reliable conclusions requires extensive sampling over an extended period.

Synthesis and Purification of 4,4'-di(n-alkyl)-2,2'-bipyridine

Brooke Andrews
Faculty Advisor: Dr. K. Nicole Crowder

Bipyridine complexes can be used to coordinate an inorganic catalyst for the electrochemical reduction of carbon dioxide, allowing for the valuable creation of new carbon-carbon bonds. When tethered to a metallic surface via a phosphonic acid, the catalyst-coated plate becomes a reusable electrode. One synthetic approach to the catalyst includes the initial attachment of alkyl chains to the bipyridine molecule. The addition of an alkyl chain to 4,4'-dimethyl-2,2'-bipyridine is facilitated by the use of an extremely strong organic base. Lithium diisopropylamide (LDA) is a sufficient base for this process as it removes a methyl proton, creating a highly reactive carbanion. Subsequent introduction of alkyl chains functionalized by primary halogens yields a mixture of singly and doubly reacted bipyridine products, which can be purified and separated by column chromatography. This process has been replicated with three different alkyl chains: terminally dibrominated long and short chains, as well as a bromophosphonate. The use of a shorter chain, 1,5-dibromopentane, prevents the dibrominated alkane from attaching to the same bipyridine molecule twice, which is possible with 1,9-dibromononane. The diethyl-2-bromoethylphosphonate starting material reduces the number of synthetic steps required to produce the phosphonic acid target compound. These three reactions have been repeated to ensure reproducible, pure products that can be used for the eventual production of functional electrodes.

Human Vs. Computer: Comparison of Performance In Solving An NP-Complete Problem

Samuel Arutyunyan
Dr. Ian Finlayson

Despite the fact that computers can solve many problems very quickly, there are certain problems, called NP-complete, that cannot be solved in a reasonable amount of time by a computer for large input sizes. The topic of my research this summer was to determine how quickly a human can solve a particular NP-complete problem called the Hamiltonian path problem. A Hamiltonian path consists of a path through a graph which visits every node in the graph exactly once. I developed a game for Android devices in which players can attempt to find Hamiltonian paths in graphs of increasing complexity. When a path is found, the name of the user and the time it took for them to complete the path will be sent to a web page where we will be able to view the results. Initial comparisons of a human player vs. a computer algorithm show that as the paths get larger, computers can take a very large amount of time to solve the problem, to the point where a human solving the problem is actually faster. Over time, we will continue to obtain data from more users as people try out the game on Google Play.

Using Independent Bernoulli Random Variables to Model Gender Hiring Practices

Kimberly Hildebrand
Faculty Advisor: Dr. Debra Hydorn

Gender bias is a problem in the workforce at large. In order for society to progress it is important that hiring practices do not use gender as a competitive factor. Hiring practices based on gender can be represented statistically using Bernoulli Random Variables and the Beta and Binomial Distributions. Using the moment generating function (MGF) of the Bernoulli and Binomial Distributions, it is possible to calculate the expected value (mean) and variance for the number of women hires for n positions. The probability generating function (PGF) of a sample size n can be used to find the probability of hiring a specific number of women (X). The PGF when solved for $P(X=0)$ reveals the probability of no women hired for n positions, while $P(X\leq 1)$ gives the probability that one or no women were hired. A computer program was used to run trials to simulate different male/female distributions using recent data on the proportion of women earning a PhD in a variety of disciplines. The simulations were used to represent hiring results for seven faculty positions. Situations where the female proportion is centered at 0.3, 0.5, and 0.7 were studied. Trials that included random proportions of women for each position were run as well. Results revealed that it is actually unusual for employers to hire one or fewer women for seven positions, which could provide evidence of gender bias.

Modeling GDP in Developing Countries

Katelyn M. Jones
Faculty Advisor: Dr. Julius Esunge

We use statistical methods to predict Gross Domestic Product (GDP) in developing countries. Intrigued by which indicators would play a role in predicting GDP, we use stepwise and best subsets methods to create multiple regression models. We focus especially on explanatory variables related to population. We work with data, provided by the World Bank, for the years 1980-2010 to predict GDP in Central African Countries. We use population, birth rate and death rate as explanatory variables, although not the only indicators we use to predict a nation's wealth.

Reflectance of Photovoltaic Cells

Philip Wahlman
Dalton Echard
Advisor: Dr. Chinthaka Liyanage

Surface reflectance plays a noticeable role in the efficiency of photovoltaic devices. This experiment made use of a white light source, a monochromator, photovoltaic cells taken from a garden solar light as the reflecting surface, a photo diode, and a lock-in amplifier in order to measure the reflectance of the solar cell. The monochromator was used to filter out all but one wavelength of light from the light source. Once the light passed through the monochromator, it struck the photovoltaic cell at a predetermined incident angle, and a portion of light is reflected while a portion is transmitted. The photo diode collects the reflected light and the photocurrent is measured by the lock-in amplifier. The reflectance is calculated by the ratio of the reflected photo current and the direct photo current. The angle of incidence is varied in order to find the angle of incidence with the lowest reflectance for the device.

Earlier Presentations

The following abstract presentations were given on July 17th to avoid conflict with presentation of the projects at a national conference

Comparing the Performance of the Intel Phi Coprocessor with CPUs and GPUs for the Brute Force Solution to the Traveling Salesman Problem

Zach Goodwyn & Jerome Mueller
Faculty Advisor: Dr. David Toth

As accelerators are integrated into many of the newest supercomputers to provide large amounts of additional processing power, selecting the appropriate one is critical for achieving the best performance. The new Intel Phi coprocessor provides more processing cores than a CPU, but less than a graphics processing unit (GPU). However, the Phi's cores do not have the limitations of a GPU's cores and can also run code written for traditional CPUs instead of requiring code written specifically for GPUs. We used the traveling salesman problem (TSP) as a benchmark application to compare the relative performance of the Phi with a contemporary GPU and CPU. A program was written to solve the TSP for the CPU and on the coprocessor that could be easily ported to run on the GPU with only minor modifications. The length of time the program took to complete on the Phi, the GPU, and the CPU was measured. The Phi performed as well as 4 CPU cores but not as well as 8 CPU cores. The GPU outperformed all 8 CPU cores by a factor of 2.5 and the Phi by a factor of 4.4.

Using Supercomputing to Search for a Cure for Histoplasmosis

Jerome Mueller & Zach Goodwyn
Faculty Advisor: Dr. David Toth

Histoplasmosis is a potentially fatal fungal respiratory disease which afflicts many people in the United States. Discovering drugs to cure or treat diseases takes years and millions of dollars in a wet lab. However, the time and financial costs of this process can be greatly reduced using a process called virtual screening. In virtual screening, a computer runs a molecular docking program to simulate how well compounds will bind to a protein. The process of virtual screening eliminates most of the compounds tested because it shows they have a low likelihood of binding to the target protein. This allows scientists to test only a minute subset of compounds in a wet lab as they search for a cure for a given disease. For virtual screening to be effective, millions of compounds must be screened against the target protein. The results of an existing virtual screen of millions of compounds were augmented by screening a set of lipids in hopes of finding one that will bind to and inhibit the Cbp1 protein and thus lead to a cure for histoplasmosis. AutoDock Vina was used to screen the lipids and predict how well they would bind to the protein. Because the lipids take much longer to screen than other molecules, a supercomputer was used to conduct the virtual screen. Some of the lipids screened are predicted to bind to the Cbp1 protein better than the other compounds from the existing virtual screen.