College of Natural Sciences and Mathematics

12th Annual Student Research Symposium

Kinetic Analysis of Vasorelaxation by β-estradiol, 2-Hydroxyestradiol, and 2-Methoxyestradiol
Sean Necessary, Tiffany Mattingly, Christi Lewis, Alisha Cooper, and Sara Weinberg
Faculty Mentor: Brent Hill

Use of the Electrical Resistance Method to Define Water Transport Pathways Across Enterocytes of *Aplysia californica*
Morgan Nixon
Faculty Mentor: Mike Moran

Do Roadways Impact Population Demographics and Nest-site Selection in a Semi-aquatic Turtle Species?
Sara Ruane
Faculty Mentor: Stephen A. Dinkelacker

Effects of Repetitive Pain Experiences During a Critical Neonatal Window Are Retained Throughout Adulthood
Pia Seballos, Heather Delahunt, Shannon Palmer, Sonja Isbell, Jason Talburt, and Adam Lucas
Faculty Mentor: Barbara Clancy

Modulation of Sodium-Hydrogen Exchanger (NHE) mRNA Levels in MCF-7 Cells Under Acidic and Hypoxic Conditions
Kyla R. Shelton, Candice Ray, and Andres Chang
Faculty Mentor: Steven W. Runge

Can the Development of Cortical Connectivity be Modeled Mathematically?
Jason Torrence, Paige Covington and Barbara Findley
Faculty Mentors: Barbara Clancy and Danny Arrigo

Patterns of Macroinvertebrate Diversity and Community Structure Across a Gradient of River-Floodplain Connectivity
Bradley S. Williams
Faculty Mentor: Reid Adams

CHEMISTRY

Using a Photolabile Precursor to Study Radical-Mediated Protein Damage
Amber Brown, Tori Green, Tara Sterrenberg
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Geometry and Sequence Dependence of H_20 Interactions with the Faces of DNA Bases
Tori O'Bannon and Garen Holman
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Synthesis and Direct Fluorination of Dendritic Monomers
Lindsay Read and Daniel Hall
Faculty Mentor: Kyle Felling

Oxidation of Organic Material Using an Electrodeless Plasma Discharge
Jeffrey Shearer and Brandon Ayers
Faculty Mentor: Karen Steelman

Metabolism of All-*trans*-Retinoic Acid in the Presence of Type-Two Diabetic Drugs
Clint Smith
Faculty Mentor: Melissa Kelley

Site Specificity and Effect of Cation-pi Interactions in DNA Crystal Structures
Mikaela Stewart and Tori O'Bannon
Faculty Mentor: Lori Isom

Ammonia Sensors, Hydrogen Storage, Methane Activation and Tripodal Nickel-Nitrogen Complexes
Christopher A. Sutton
Faculty Mentor: Patrick J. Desrochers

SEIRA and SERS Analysis of Para-Nitrobenzoic Acid and Nitroaniline Isomers
Mark Viegas, Chen Wang, Krissy Posey, Merritt Smith, Jacob Boucher, Bridgette Bridges, Brittany Carpenter, Steve Baker, and Kaitlyn Stambaugh
Faculty Mentor: Don Perry

COMPUTER SCIENCE

Optimal Scheduling Algorithms for Large Scale Multi-Objective Emergency Management
Meaghan Dellar
Faculty Mentor: Chenyi Hu

Internet-based Generic Architecture for Distributed Heterogeneous Robotic Systems
Mike Moncrief, Scott Dancer, Nathan Hotchkiss, and Dewan Rahman
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An Object-Oriented Software Toolbox for Interval Linear Algebra
Micheal Nooner
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Building an Experimental Globus-Based Grid Computing System
Vineet Saini
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Investigation on the GridFTP File Transfer Protocol for Grid Computing
Yun Zhou
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Knot Theory: Generalizing the Arf Invariant
Rachel Courtney, Stephanie Lanier
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Evaluating Unit Hydrograph for Stream Flow
Akhil Mehta and Chase Ransom
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Marimba Bar Tuning and Young's Modulus
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Rat-holes in Highly Friction Granular Materials?
Jason Torrence
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PHYSICS AND ASTRONOMY

Unraveling the R-Process: A Second Site for Lighter N-Capture Elements?
Tuesday D. Brown and E. Marilea Jones
Faculty Mentor: Debra L. Burris

Scanning Electron Microscope Studies of Leg Bone Sample: Influence of Simulated Microgravity in Adult Male Mice
Ashley Brown
Faculty Mentor: Rahul Mehta

Chaos in Electric Circuits
Travis Hoggard, Katharina Ochterbeck, and Katie M. Reynolds
Faculty Mentor: Stephen R. Addison

Symmetry Analysis of the Quantum Harmonic Oscillator
Jason House
Faculty Mentor: Balraj Menon

ABSTRACTS

BIOLOGY

Induction of Apoptosis in MCF-7 Human Breast Cancer Cells by [dppeNiCysEt^{+}]Cl^{-}

Kyle B. Basham, Tony Manning
Faculty Mentors: Steven W. Runge and Patrick Desrochers

Apoptosis, or programmed cell death, is an essential mechanism for the development and maintenance of multi-cellular organisms and is the form of cell death most commonly caused by cancer therapies. The pathways of apoptosis are numerous and can be triggered by many diverse stimuli. A new method of inducing apoptosis may exist with the development of metal phosphine complexes. Many of these complexes have been found to have antitumor activity, with Ni(II) bis-(phosphine) complexes being among those showing promising results. The specificity of [dppe] ligated nickel compounds to bind cysteine and homocysteine is thought to give it these potentially chemotherapeutic qualities. In this study, MCF-7 human breast cancer cells will be exposed to the [dppeNiCysEt^{+}]Cl^{-} compound. Visual observations using phase contrast microscopy were taken daily to inspect for cellular death. The lowest effective dose that kills the cells within 72 hours will be stained with Annexin V-FITC and propidium iodide, the control agent, and visualized using fluorescent microscopy. Green cells will be interpreted as apoptotic while green cells having red nuclei will be scored as necrotic. Healthy cells will not fluoresce. If the dying cells are apoptotic, further experiments will be conducted to determine whether the [dppeNiCysEt^{+}]Cl^{-} is effective under conditions similar to that found in solid tumors. Acid-adapted cell lines in a hypoxic environment will be exposed to the compound and tested again for apoptosis. If cell death occurs in the form of necrosis, alternate forms of treatment will be examined to insure apoptosis cannot be initiated by the compound. By determining the method of cell death caused by [dppeNiCysEt^{+}]Cl^{-}, we will gain a further understanding of the effect of ligated metal compounds on human tumor cells. Future experiments may then involve the designing of specific, tumor-searching, nickel ligated compounds to induce apoptosis *in vivo*.

An Analysis of Temporal Changes in Fish Communities Utilizing Off Channel and Backwater Habitats of the Arkansas River

Robert Clark
Faculty Mentor: Reid Adams

Large rivers worldwide have been modified for flood control and to facilitate commercial navigation to the point that natural processes that regulate them (e.g., seasonal flooding) are absent or diminished in magnitude. These alterations have had negative impacts on the river floodplain by disconnecting the main channel from their backwaters and floodplain habitats. Mitigation to the Arkansas River Navigation channel has been recently proposed to increase the depth of the main channel to allow for increased commercial transportation. The impacts of this proposed mitigation on the Arkansas River fish communities are currently unknown. Due to the proposed mitigations, there is a need to gather more baseline data on fish communities of the Arkansas River. Previous research conducted on the Arkansas River by Buchanan (1976) focused primarily on the main channel. My research will focus on temporal changes of fish use in off channel and backwater habitats. Each selected site will be sampled three times over a period of approximately three months. Each sampling period corresponds with water temperatures at which different species of fish move into spawning habitats. This research will help conservationists and resource managers better understand the impacts that alterations to the main channel have on the fish communities of the Arkansas River.

Thermoregulation in Alligator Snapping Turtles (*Macrochelys temminckii*): Correlates of Habitat Use, Sex, and Reproduction

Christopher A. Howey
Faculty Mentor: Stephen A. Dinkelacker

Turtles rely on thermoregulation to increase and maintain a body temperature that will permit daily activities. For instance, elevated body temperatures are necessary for a variety of reasons including feeding, foraging, growth, maintenance of illness or injury, digestion, and reproduction. Among these different activities, reproduction is the only one that may be dependent upon sex and reproductive status. Since the body temperature of a reptile relies heavily on surrounding environmental temperatures, habitat selection should differ between males and females. Furthermore, habitat selection should differ between gravid females and non-gravid females. Whereas most freshwater turtles leave the water to bask, the alligator snapping turtle (*Macrochelys*

using nonparametric multidimensional scaling and multi-response permutation procedures. In addition, habitat selection will be determined through pairwise *t*-tests comparing turtle locations to random locations. Inferences can then be made on whether thermoregulatory requirements influence habitat use and selection.

Effects of Estrogen and Its Metabolites on Breast Cancer Cell Lines

Jamie Johnson and Ben Szpila
Faculty Mentors: Brent Hill and Steven Runge

Estrogen has been shown to have tumorigenic effects when used in hormone replacement therapies. However, 2-Methoxyestradiol (2MEOH), a metabolite of estrogen, has been shown to have anticancer properties. The purpose of our study was to investigate the effects of estrogen and its metabolites on human breast cancer cells. MCF-7 (estrogen receptor positive) and Hs578T cell lines (estrogen receptor negative) cells were exposed to 2-estradiol, 2-hydroxyestradiol (2HEOH), and 2MEOH under normoxic and hypoxic ($1\%O_2$: $5\%CO_2$: $94\%N_2$) conditions. Cells were counted to determine the proliferative

Language (PHP) allow for real-time, comparative neurodevelopmental conversions, including predicted dates of neural events for which empirical data are currently unavailable. The use of this web site will help to provide greater precision to medical professionals who need to estimate timing of neurodevelopmental events in the human fetus. The site will also provide precision to biomedical researchers who need to do the same for laboratory species or those who wish to identify comparable developmental timing in different mammalian species. (*Support Contributed By: NIH P20RR-16460 INBRE, UCA CNSM, DEPARTMENT OF BIOLOGY)*

2-Methoxyestradiol-Induced Coronary Artery Relaxation in Two Different Age Groups of Pigs

Adam McCall and Matt McShane
Faculty Mentor: Brent Hill

β-estradiol (i.e. estrogen) is sequentially converted to 2-hydroxyestradiol and 2-methoxyestradiol in the liver, bloodstream, and the wall of arteries. The functional significance of these metabolites of β-estradiol has not been clearly defined. Therefore, the purpose of our study was to compare the relaxant effects of the β-estradiol metabolite,

2-Methoxyestradiol Mediates a Greater Coronary Arterial Relaxation Response than 17β-Estradiol in Old Female Pigs

Matt McShane and Ben Szpila
Faculty Mentor: Brent Hill

The protective effects of 17β-estradiol against coronary artery disease may partially be due to the action of its metabolites. The objective of this study was to determine the arterial relaxation induced by the metabolites of 17β-estradiol using coronary arteries obtained from old female Yorkshire retired breeding pigs (3-4 years old). These pigs demonstrated reproductive failures and/or a decline in litter size. The right coronary artery was dissected from each heart, and then sectioned into 3 mm rings which were suspended in organ baths. The rings were pre-constricted with a 60mM K^+ solution before generating a concentration-response relationship (10-6 to 10-4M) to 17β-estradiol, 17α-estradiol, 2-hydroxyestradiol (2-OHE), and 2-methoxyestradiol (2-MeOH). Arterial relaxation was initially demonstrated at 10-5M for all the agonists; however, only the 2-MeOH-induced relaxation (27.47±5.90%) was greater than the other agonists at this concentration. The maximum relaxation achieved at 10-4M was: 2-MeOH (90.40±3.48%) > 17β-estradiol (62.85±8.00) > 2-OHE (49.30±11.12) > 17α-estradiol (37.41±4.25). The selective estradiol receptor antagonists (10-5M), tamoxifen and ICI 182,780, did not effect the relaxation response to 2-MeOH. These data contrast results obtained using coronary arteries from market-age pigs (6-9 months) in which the 17β-estradiol-induced relaxation occurred at much lower concentrations; thus suggesting that the arterial responsiveness to 17β-estradiol decreases with age. In addition, our results suggest that the potent 2-MeOH-induced relaxation is not mediated by the "classical" estradiol-mediated receptor mechanisms in old pigs.

Kinetic Analysis of Vasorelaxation by β-estradiol, 2-Hydroxyestradiol, and 2-Methoxyestradiol

Sean Necessary, Tiffany Mattingly, Christi Lewis, Alisha Cooper, and Sara Weinberg
Faculty Mentor: Brent Hill

The incidence of coronary artery disease (CAD) increases dramatically in women following menopause. This increase in CAD has been linked to the decline in 17β-estradiol (i.e. estrogen) levels in the bloodstream. One of 17β-estradiol's protective effects against CAD is its ability to relax and dilate arteries. The purpose of our study is to evaluate the ability of 17β-estradiol and its breakdown products, 2-methoxyestradiol and 2-hydroxyestradiol, to relax those arteries that provide blood to the heart (i.e. coronary arteries). Coronary arteries were dissected out of hearts obtained from 3-4 year-old retired breeding sows. The arteries were sectioned into rings and suspended in organ

baths. These arterial ring segments were exposed to a depolarizing 60 mM KCl solution, thus causing a contraction. While in its contracted state, the rings were exposed to 3x10-5 M 17β-estradiol, 2-methoxyestradiol, 2-hydroxyestradiol, or the ethanol vehicle for 60 minutes. The tone of the artery (contraction and relaxation) was recorded by the Dataq acquisition system. The time for the artery to relax (5, 10, 25, 50, 75, and 100%) in response to 17β-estradiol or its metabolites was determined. Preliminary analysis suggests that 17β-estradiol takes longer to cause a relaxation response than its

Do Roadways Impact Population Demographics and Nest-site Selection in a Semi-aquatic Turtle Species?

Sara Ruane
Faculty Mentor: Stephen A. Dinkelacker

Although the protection of wetlands is of critical importance to the survival of many species, the conservation of upland areas surrounding wetlands is often not legally required or is simply overlooked. Many species of turtles require upland habitats to successfully complete their life cycles. For example, the Blanding's turtle (*Emydoidea blandingii*) is a species that depends upon upland habitats for successful nesting and ultimately, population recruitment. Currently, it is unknown how nest-site selection and the demographics of remote populations compare to populations residing in wetlands bisected by man-made constructs such as roads. Beginning summer 2005, Blanding's turtles were trapped in remote and roadside sites in western Nebraska. Age, sex, and morphometric data were recorded for each individual captured. Gravid females had a transmitter attached and were followed to nests. Preliminary analysis of the data suggests that populations in remote habitats have female biased populations and greater proportions of adults, while populations alongside roads have a more varied sex ratio and a higher proportion of juveniles. The data also suggests that females at remote sites travel

follow rules of simple diffusion while other connectivity patterns may be modeled mathematically by ray paths through variable density media in the direction of the development gradient. If this proves to be true, it may help explain how and why developing axons focus on, and concentrate in, characteristic remote brain regions. Further, it may help explain the mechanics of evolutionary development of the mammalian brain.

Patterns of Macroinvertebrate Diversity and Community Structure Across a Gradient of River-Floodplain Connectivity

Bradley S. Williams
Faculty Mentor: Reid Adams

We have only recently begun to realize the importance of flood events in the functioning of floodplain ecosystems. During floods, the hydrologic connection between a river and its floodplain has been shown to stimulate primary and secondary productivity through the exchange of dissolved nutrients and organic matter. Hydrologic connectivity may also be a strong mechanism influencing the community structure and diversity of aquatic organisms by increasing habitat heterogeneity. River management practices that facilitate commercial transport and control seasonal flooding disrupt the timing, duration, and ability of natural flood pulses to inundate floodplains. The importance of maintaining a natural level of hydrologic connectivity in regulated river floodplains has become an important area of research, but only a limited number of studies have examined the effects of connectivity on macroinvertebrate diversity and community

presence of UV light. Isomers were formed when *t*-RA was exposed to UV light in methanol, ethanol, and hexane. However, some isomers produced initially experienced further reaction, leading to a decrease in concentration of the initial isomers at 10, 15, and 20 minute time periods. Those reactions appear to occur faster in small polar solvents, with non-polar bulkier solvents having a slower rate. While the initial isomers were detected after exposing the hexane samples to UV light for 20 minutes, those same isomers were not detected in the methanol or ethanol samples that were exposed over the same period. Our data suggests that solvent polarity and size plays a significant role in all-*trans*-retinoic acid isomer production.

Accelerator Mass Spectrometry Measurements of Calcium Oxalate Accretions Associated With Spanish Rock Paintings

Jacque DuPriest
Faculty Mentor: Karen Steelman

Determining the Kinetics of Linkage Isomerization: Optimizing an Undergraduate, Inorganic Chemistry Laboratory Experiment

Daniel Hall and Lindsay Read
Faculty Mentor: Kyle Felling

The advanced inorganic chemistry laboratory is a place for students to combine knowledge gained from all their other laboratory courses. The goal of the inorganic laboratory is to give students experience in the use of a range of techniques that are typical for the synthesis and characterization of inorganic compounds and to give them experience in preparing various classes of inorganic compounds. It is recommended that the methods of synthesis, purification, and characterization be synergized into common experiments. The developed laboratory allows the student to synthesize a series of common, inorganic coordination compounds, purify them through recrystallization/ filtration, and characterize the compounds through NMR, IR and UV/Vis spectroscopy. This lab also allows for study of the kinetics of conversion from an unstable linkage isomer to a more stable form. Synthetic approaches and difficulties with previously published procedures for the kinetics portion of this laboratory will be presented.

Synthesis of 3rd Generation Dendrimers as Chemosensors

Garen Holman, Hua Mao, Robert E. Gawley
Faculty Mentor: Robert E. Gawley (UARK)

DNA Bending Observed in DNA/Protein Complexes is Correlated with Phosphate Collapse in the Vicinity of Cationic Protein Residues

Courtney Huff and James Lewis
Faculty Mentor: Lori Isom

DNA deformation is crucial in many fundamental biological processes such as DNA packing, proper functioning of the immune system, gene activation, and DNA mutation repair. In this project we tested the theory that cation interactions with DNA phosphate groups results in partial charge neutralization inducing DNA bending. We used X-ray crystal structures of protein/DNA complexes to investigate the influence of cations on DNA structure. Unlike monovalent ions, the position of cationic side chains, such as lysine and arginine are quantifiable and so their location with respect to DNA phosphate oxygens can be calculated. We selected DNA/protein crystal structures with a resolution of 2.7 Å or higher and screened for phosphate crowding around high densities of cationic protein residues. The structures obtained were then used to investigate the relationship between phosphate crowding, cation density, and the direction of DNA bending. Analysis of 121 structures led to results suggesting that phosphate crowding is related to cation density. A positive correlation value (0.321 ± 0.070) was calculated for DNA/protein complexes containing DNA that bends toward the bound protein, while a negative value (-0.215 ± 0.139) was observed for complexes with DNA bending away from the protein. Complexes containing unbent DNA have a correlation close to zero (0.018 ± 0.076). The observed correlations support our hypothesis that a relationship exists between phosphate crowding, cation density, and DNA bending.

Radiocarbon Measurements of Black Carbon in Mexico City Aerosol

Amanda MacMillan and Megan McQueen
Faculty Mentor: Karen Steelman

We report measurements of radioactivity in fine aerosol in one of the largest megacities in the world, Mexico City. Naturally occurring radionuclides enable us to study the transport of ozone and aerosol in the troposphere. Radiocarbon measurements for carbonaceous aerosol can indicate sources of carbon as either from fossil or biomass derived carbon sources. Samples were collected on quartz fiber filters by using cascade impactors and high-volume air samplers on the rooftop of the main laboratory of El Centro Nacional de Investigación y Capacitación Ambiental (CENICA) during the month of April 2003. Radiocarbon levels were determined by accelerator mass spectrometry and demonstrated a 70% modern biogenic-to-fossil ratio indicating that carbonaceous aerosol was from three sources: fires in the Yucatan; oxidation of monoterpenes and sesquiterpenes emitted from a nearby fruit-drying facility; and trash burning within the city.

nickel site. Phosphorus-rich environments are expected to favor reduced nickel. Nickel reduction and cysteine protonation are two key steps in functional hydrogenase activity.

An Investigation of DNA Damage Induced by the Chemotherapeutic Drug Cyclophosphamide

Akhil Mehta, Jake Smith

from a centroid were isolated. These water-pi interactions were then analyzed for sequence specificity, major/minor groove patterns, and average distance and angle of interaction. According to these criteria, water-pi interactions were found in all structures analyzed. The water-pi interactions occurred most often with adenine in the major groove and thymine in the minor groove. When an AATT sequence occurred, a water was found to be interacting in the minor groove with bases on both chains. In the major groove, these interactions only occurred with the side of the base facing the 3' end of the DNA, and they only occurred with the side facing the 5' end of the DNA in the minor groove. The interacting waters formed a ribbon in the major groove and a spine in the minor groove. The water-pi interactions also showed evidence of base unstacking. It is concluded that water-pi interactions are common in DNA. These interactions are sequence dependent and interact with only one side of a base depending on steric effects.

Synthesis and Direct Fluorination of Dendritic Monomers

Lindsay Read and Daniel Hall
Faculty Mentor: Kyle Felling

Dendrimers are highly branched molecules consisting of a central core from which regular repeat units emanate to form a globular, monodisperse macromolecule. Fluorinated dendrimers are a class of molecules, which have very unique properties compared to normal dendrimers because of the strong electron-withdrawing influence of the fluorine atoms. They have considerable potential applications as optoelectronic materials, surfactants, solvents, and drug delivery agents. Direct fluorination, a process in which elemental fluorine is used to replace hydrogen atoms in organic/inorganic compounds with fluorine atoms, has many advantages for commercial and large-scale production of fluorocarbons with high yields. In this study, the perfluorinated analogues of polyether, sulfur-containing and poly (propylene imine) dendrimer frameworks are produced using the Exfluor-Lagow direct fluorination technique. Subsequent characterization is also discussed.

Oxidation of Organic Material Using an Electrodeless Plasma Discharge

Jeffrey Shearer and Brandon Ayers
Faculty Mentor: Karen Steelman

We utilize the properties of oxygen plasmas, electrically excited oxygen gas ignited with a radio frequency generator, to collect organic carbon from archaeological materials for radiocarbon dating. We produce a plasma glow when current is delivered to a gas by means of two external electrodes, making our plasma process an electrodeless discharge. Free electrons are accelerated to sufficient energies to cause ionization in a small fraction of gas molecules and atoms. Electrons gain kinetic energy from the oscillating electric field, while the temperature of the gas components is increased by elastic collisions between electrons and the gas. Electrons are thermally isolated from the gas components

by the very large mass difference. Electrically excited oxygen therefore gently converts organics to carbon dioxide and water, without decomposing carbon-containing inorganic minerals. Collected carbon dioxide is measured using accelerator mass spectrometry to determine radiocarbon age. Samples studied include paint samples from prehistoric cave paintings from Arkansas and rock from purported mammoth rub sites in California.

Metabolism of All-*trans*-Retinoic Acid in the Presence of Type-Two Diabetic Drugs

Clint Smith
Faculty Mentor: Melissa Kelley

Retinoids are vitamin A analogs that control a variety of cellular processes through binding to nuclear retinoid receptors. Two biologically active retinoids are all-*trans*-retinoic acid (*t*-RA) and 9-*cis*-retinoic acid (9-*cis*-RA). These retinoids act as ligands for retinoic acid receptors (RAR). These receptors form heterodimeric partners with other receptors including peroxisome proliferators-activated receptor gamma (PPARγ). When RAR and PPARγ dimerize, they initiate the transcription of proteins that decrease blood sugar levels. Thiazolidinediones (TZDs) are a class of drugs that are widely used to treat type-two diabetes. TZDs have two biochemical functions. First, TZDs act as ligand for PPARγ. Secondly, they are inhibitors of cytochrome $P_{450,}$ which is responsible for the metabolism of *t*-RA. This project investigates the metabolism of *t*-RA in the presence of TZDs. Using Sprague-Dawley male rat microsomes, which contain the cytochrome P_{450} family of enzymes, metabolism of *t*-RA was examined in the presence and absence of TZDs. The goal of our research is to determine if metabolites of *t*-RA are altered in presence of TZDs.

Site Specificity and Effect of Cation-pi Interactions in DNA Crystal Structures

Mikaela Stewart and Tori O'Bannon
Faculty Mentor: Lori Isom

Cation-pi interactions are a type of cation-induced DNA distortion that pulls bases out of the helical stack and into the major groove where a bound Mg^{2+} ion or waters of its bound hydration shell interact with the exposed aromatic face of the unstacked base. Many high resolution DNA structures have been deposited in the PDB since the initial publication describing DNA cation-pi interactions in 2DNA and 2 RNA structures (Isom, et al., Biochemistry, 1998). A survey of the Nucleic Acid Database (NDB) produced 10

distances less than or equal to 5.0 A and angles less than or equal to 50 degrees were considered cation-pi interactions. Using this procedure, cation-pi interactions were detected in 9 of the 10 high-resolution structures analyzed, including the surprising discovery of cation-pi interactions between DNA bases and monovalent thallium ions (PDB 1JGR). These interactions were found to induce DNA distortion including base unstacking in many of the structures. Based on these data, we conclude that cation-pi interactions are common between cations and DNA bases and that these interactions do, indeed, induce DNA distortion.

Ammonia Sensors, Hydrogen Storage, Methane Activation and Tripodal Nickel-Nitrogen Complexes

Christopher A. Sutton
Faculty Mentor: Patrick J. Desrochers

Hydrogen storage and methane activation represent significant challenges for the increasing use of these simple gases as commercial energy sources and industrial raw materials. Research in this laboratory on tripodal (C_{3v}) N_3NiX complexes has produced results suggesting potential solutions to both of these challenges. To date, X in the above complexes includes Cl^-, Br^-, I^-, BH_4^-, NH_3, and ^-SPh. The N_3 nitrogen donor atoms are provided by the facial tridentate chelate, Tp* (hydrotris(3,5-dimethyl-1-pyrazolyl)borate). An example of the interaction of Tp*NiX with ammonia involves its rapid binding of the gas, forming $[Tp^*Ni(NH_3)_3^+][X^-]$. This ammonia gas uptake is reversible; ammonia is released with gentle heating. These solid $[Tp^*Ni(NH_3)_3^+][X^-]$ compounds are interesting both as precursors to the elusive fluoride derivative (Tp*NiF) and as the basis for efficient ammonia sensor/storage materials. The electronic structure of the halide and borohydrj ET Q q 0.23999999 0 0 -0.ea01228 1498e0 0 - 1 Tu1h These solid [Tp*Ni(NH

from 1-12 nanometers thick as measured by reference to a geometrically equivalent quartz crystal microbalance. Infrared spectra were obtained in transmission mode. The presence of the thin silver film serves to enhance the infrared signal of many organic molecules that are deposited on the silver layer. The best enhanced spectra were obtained with seven nanometers of silver. PNBA NO_2 and COO^- stretching modes exhibited the most intense SEIRA enhancement. These bands were symmetric and enhanced by about x50 in comparison to thick PNBA layers on clean calcium fluoride.

SEIRA studies were performed with o-, m-, and p-nitroaniline (O-, M-, P-NA). Most of the M-NA infrared bands were strongly enhanced in the SEIRA spectra, but O-NA and P-NA exhibited no SEIRA. Opposing trends are being observed in surface-enhanced Raman spectroscopy (SERS) experiments for the nitroaniline isomers. The enhancement seen in the vibrational spectra of the nitroaniline isomers are attributed to a combination of resonance and geometric absorption properties of the different isomers.

COMPUTER SCIENCE

Faculty Mentor: Chenyi Hu

Natural disasters may cause large-scale evacuations and aftermath relief efforts. Most recently, hurricanes Katrina and Rita hit the gulf coast and caused huge losses of both human lives and properties. A study on large scale emergency management is much needed. In this research project, we apply optimal scheduling algorithms for large scale emergency management with multiple objectives.

To accomplish the above, we have studied existing models related to task management such as weighted graph, acyclic directed graph, topological order, and flow network. We further construct models that include multiple sources, destinations, and objectives. By applying problem solving strategies such as greedy approach, divide and conquer, dynamic programming and others, we try to establish algorithms that provide solutions for multiple objective optimization problems involving multiple sources and destinations. These algorithms are being implemented as software tools for validating the designed algorithms. The software tools can also be applied to simulate various multi-objective emergency management tasks.

Faculty Mentor: Han-Chieh Wei

In robotic systems, there are a variety of tasks that can take advantages of using a group of robots to perform coordinated activities. In the past decade, the trend of robotic research has been focused on the coordination of multiple distributed robots and cooperation with human controller. These robots are equipped with different capabilities, hardware, software, and different communication interfaces. The control devices may vary from desktop computers, laptops, palm PCs, to even voice controllers. These heterogeneities introduce complicated communication and integration problems for robot control and coordination. There is extensive research on control, management, and coordination of heterogeneous robotic systems. Most of the research and projects focus on different features of distributed robotic systems for specific applications. In particular, different applications have different needs, which can be satisfied with special system architectures. Instead of these task-oriented architectures, it is desirable to have a general purpose system which allows for flexible addition/change of behaviors and resources to facilitate the requirements for different applications. In this project, we design and implement the internet-based wireless-connected Generic Distributed Heterogeneous Robotic System architecture to serve various applications and tasks.

Faculty Mentor: Chenyi Hu

Interval Computing was introduced in the 1960's by Dr. Moore. It has been successfully applied by many people in various applications. To make intervals easy to use, software has been developed. However, existing software tools tend to either be highly specialized or they do not support object-oriented paradigm. The software toolbox we developed attempts to remedy this by creating a truly general purpose object-oriented software library that is easy to use, easy to install, and cross platform compatible. This software

dependencies on third party applications. Also, it has no dependency on hardware rounding; this makes it easy to port to other platforms. IntBLAS is well documented, easy to use, with no complicated runtime or compilation issues. Finally, it adheres to the interval BLAS standard, making it the only object-oriented implementation so far to explicitly do so.

Faculty Mentor: Qiang Duan

Grid computing is a new paradigm for distributed computing. It has had significant impacts on many areas of computing. It is changing the way that scientists and engineers do computing and the society manages information in general. Grid computing technologies have led to the development of a global Grid community. The Globus Toolkit is the *de facto* standard for building grid computing systems and services by the community currently. In order to obtain deeper understanding about Grid computing technology and the Globus Toolkit, we are building an experimental Globus-based grid in our network laboratory. This Grid can be used for both education and research purposes. Due to the complexity of the grid computing technology and the lack of well-organized documentation for the Globus Toolkit, it has been a challenge to build the experimental Globus-based grid.

Faculty Mentor: Qiang Duan

Grid computing is an emerging computing model that enables the clustering of a wide variety of networked computing resources, such as computers, storage systems, data sources, and special devices. Then, these devices can be utilized as a unified resource. Networking forms the foundation of grid computing systems. Data communication across wide area networks plays a critical role in a computing grid. The newly developed GridFTP, an extension of the Internet File Transfer Protocol (FTP), has been widely employed as the data transfer mechanism in Grid computing systems.

The performance of GridFTP has a significant influence on the performance of Grid computing. In this project, we investigate the GridFTP protocol and exam if it meets the performance requirements of Grid computing. We have studied the working mechanisms of GridFTP and setup a Grid prototype for GridFTP. We plan to test GridFTP on this prototype and analyze its performance, including throughput, reliability, security, and scalability.

MATHEMATICS

Knot Theory: Generalizing the Arf Invariant

Rachel Courtney, Stephanie Lanier
Faculty Mentor: Fred Hickling

Mathematical Knot Theory involves using and finding techniques to distinguish knots and links. Typically, these are called invariants; we are interested in the Arf Invariant. The Arf Invariant is calculated as

$$\sum_{i,j=1}^{n} Lk(\alpha_i, \alpha_j^+) \cdot Lk(\beta_i, \beta_j^+).$$

Here the α's and β's form a basis for curves on a Seifert surface for the knot. *Lk* is the linking number between the curves in question. When all these linking numbers are zero, we generalize this using higher order linking numbers. For example, the generalized third order Arf Invariant is:

$$\sum_{i,j,k=1}^{n} \overline{\mu}(\alpha_i, \alpha_j, \alpha_k) \cdot \overline{\mu}(\beta_i, \beta_j, \beta_k).$$

In general, if all linking numbers of order *(n-1)* vanish, then the n^{th}-order Arf Invariant is defined.

Faculty Mentor: David Peterson

Given excess rainfall "*i*" in inches, the total observed discharge "*q*"in ft^3/sec can be estimated by using the convolution equation $Q(t) = \int_0^t I(t-\tau)\, U(\tau)\, d\tau$, where *u* is the theoretical flow in response to an instantaneous 1 inch runoff event. We will present a useful formula for *u*.

Marimba Bar Tuning and Young's Modulus

Michael Schelkopf
Faculty Mentor: David Peterson

The eigenvalues for a rectangular bar are not harmonic, so reshaping the bar is required to get the eigenvalues to be harmonic. Young's modulus has to be calculated because it is required in order to calculate these eigenvalues. Young's modulus is usually calculated

for homogeneous materials, but we can find an equation that calculates Young's modulus for a non-homogeneous material such as wood.

Rat-holes in Highly Friction Granular Materials?

Jason Torrence
Faculty Mentor: Danny Arrigo

Granular materials are extensively used in many industries around the world. Since many national economies are critically dependent on agricultural and mining industries that involve the handling of granular materials, it is therefore necessary to understand the physical behaviors of these types of materials. The ability of granular materials to flow through a converging hopper is a very important application to many industrial processes. However, the flow of material is often prematurely stopped and a “rat-hole” is formed. This is the general term used to describe stable cavities that frequently occur in storage hoppers, whose formation prevents further material from falling through the outlet. Our recent investigations have revealed that the partial differential equations used to model the stress distribution within a rat-hole can be greatly simplified in the case of highly frictional materials. The goal of our research is to exploit our recent results to predict stress distributions in a variety of different rat-hole geometries frequently seen in experiment.

PHYSICS AND ASTRONOMY

Unraveling the R-Process: A Second Site for Lighter N-Capture Elements?

Tuesday D. Brown and E. Marilea Jones
Faculty Mentor: Debra L. Burris

Theoretical models for the rapid neutron-capture process (r-process) reproduce the observed abundances of elements beyond Barium (Z=56). No existing model provides an adequate explanation of the formation of lighter neutron-capture elements (Z= 30-55). The existing observational data of the lighter n-capture elements Strontium, Yttrium, and Zirconium, though sparse, indicates that the existence second process may be required to explain their formation (Burris et al 2000, Sneden and Cowan 2003 and others). Recent HST observations of the element Germanium (Cowan et al 2005) have provided another source of data and another source of consternation. If the Ge is compared to known the r-process element Europium, it clearly shows no correlations. Additionally, if it is

Symmetry Analysis of the Quantum Harmonic Oscillator

Jason House
Faculty Mentor: Balraj Menon

Symmetry group methods are applied to the quantum harmonic oscillator to:

1. generate new classes of time-dependent, closed form solutions of the quantum oscillator, and

2. investigate the variational symmetries of the quantum oscillator.

We are able to show that the coherent state and squeezed state solutions of the quantum harmonic oscillator are a special subset of the obtained solutions. The significance of the variational symmetries are discussed by applying Noether's theorem, which proves the existence of a one-to-one correspondence between variational symmetries and local conservation laws.