The Midstates Consortium for Math and Science presents

Undergraduate Research Symposium

Physical Sciences, Mathematics and Computer Science

November 15-16, 2024
Washington University in St. Louis

Beloit College - Carthage College - Colorado College - Grinnell College
Gustavus Adolphus College - Hope College - Knox College
Lawrence University - Macalester College
St. Olaf College - University of Chicago
Washington University in St. Louis

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Undergraduate Research Symposium for Physical Sciences, Mathematics and Computer Science
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Program Schedule

Friday, November 15		
1:00 – 5:30 pm	Check-in at Clayton Plaza Hotel 7750 Carondelet Ave, Clayton, MO 63105 (314) 726-5400	Clayton Plaza Lobby
5:30 – 5:40 pm	WELCOME Richard Mabbs, Associate Professor Department of Chemistry Washington University in St. Louis Pamela Kittelson, Director Midstates Consortium for Math and Science Professor, Gustavus Adolphus College	Clayton Plaza Hotel Grand Ballroom
5:40 – 6:25 pm	KEYNOTE LECTURE ***The Power of Empty Space: Adventures in the Nanoscience of Metal-Organic Frameworks*** Mark D. Allendorf Senior Scientist at Sandia National Laboratories	Clayton Plaza Hotel Grand Ballroom
6:30 – 7:30 pm	Dinner Buffet	Clayton Plaza Hotel Grand Ballroom
7:45 – 8:30 pm	JANET ANDERSON LECTURE ***Changing Perspectives in Analytical Chemistry*** Ken Brown Professor of Chemistry Hope College	Clayton Plaza Hotel Grand Ballroom
Following lecture	Group Picture	

WiFi Access: WUSTL-Guest-2.0

	Saturday, November 16	
Starts at 6:30 am; avoid the 7:45 rush	Breakfast at hotel	Clayton Plaza Lobby
8:00 – 8:15 am	Load buses and vans. Bring luggage if leaving on Saturday. There is a secure room for luggage and posters at the meeting	Clayton Plaza Lobby
8:30 – 9:00 am	Set-up for poster session 1	Rettner Gallery and Wrighton
9:00 – 10:15 am	Session 1 Poster Presentations (n = 21)	Rettner Gallery & 3rd floor hallway
10:15 – 10:30 am	Remove posters Check set-up & load oral presentations	Coffee & tea near Wrighton 300
10:30 – 11:30 am	Session I Oral Presentations	
	Session I.A: Moderator Murphy Brasuel	Wrighton 201
	Session I.B: Moderator Paul Fischer	Wrighton 250
	Session I.C: Moderator Katherine Harris	Wrighton 301
11:30 am – 12:30 pm	Lunch. Student session: Applying to and Life in Graduate School	Holmes Lounge
	Lunch. Faculty social	Holmes Lounge
12:30 – 12:45 pm	Set-up posters for Session 2	Rettner Gallery and Wrighton Hall
12:45 – 2:00 pm	Session 2 Poster Presentations (n= 22)	Rettner Gallery & 3rd floor hallway
2:00 pm – 2:15 pm	Break. Remove posters. Check set-up for and load oral presentations	Coffee & tea near Wrighton 300
2:15 pm – 3:15 pm	Session II Oral Presentations	
	Session II.E: Moderator Michael Gerten	Wrighton 201
	Session II.F: Moderator Graham Sazama	Wrighton 250
	Session II.G: Moderator Kristen Burson	Wrighton 301
3:15 pm – 3:30 pm	Break. Set-up for Poster Session 3	Coffee & tea near Wrighton 300
3:30 pm – 4:45 pm	Session 3 Poster Presentations (n = 19)	Rettner Gallery & 3rd floor hallway
4:45 pm – 5:00 pm	Meeting Concludes**.** Remove posters**.** Take boxed dinners to go**,** depart for airport or drive, return to hotel if staying Saturday night. Complete online evaluations	

Keynote Address

The Power of Empty Space: Adventures in the Nanoscience of Metal-Organic Frameworks

Dr. Mark D. Allendorf
Senior Scientist at Sandia National Laboratories

Abstract: Metal-Organic Frameworks (MOFs) are nanoporous materials with record surface areas and pore volumes. They have a "Tinkertoy" architecture: new structures can be designed by assembling organic ligands and metal ions, which are analogous to the sticks and corner connectors of the iconic toys. This is a chemist's dream-come-true, creating a synthetic playground in which the design rules are well defined. Although much of the early excitement about MOFs concerned their use in gas storage, separations, and catalysis, it is now clear that there are optoelectronic applications as well. I will provide a brief MOF tutorial and an overview of my research to develop them for applications in electronic devices, energy storage, and sensing. In addition to the science, I will also present some personal anecdotes that have made my career at a national laboratory incredibly rewarding. The lessons learned are useful guideposts for those considering a career in science as well as early-career researchers.

About: Dr. Mark D. Allendorf is a Senior Scientist at Sandia National Laboratories in Livermore, California and Co-Director of the DOE Hydrogen Materials – Advanced Research Consortium (HyMARC). He obtained a B.A. in chemistry from Washington University in St. Louis and attended graduate school at MIT and Stanford, where he obtained his Ph.D. in inorganic chemistry. At Sandia, his research focuses on the fundamental science and applications of metal-organic frameworks (MOFs) and on hydrogen storage. Current interests include metal hydrides and MOFs for hydrogen storage, MOFs for electronic devices, and machine learning for materials discovery. His research has generated over 240 publications (H index 75, more than 35,000 citations), as well as fourteen patents. During his career he has mentored 28 postdocs and numerous undergraduate and graduate student interns. In 2022 he was appointed Benedict Distinguished Visiting Professor of Chemistry at Carleton College (Northfield, MN), where he taught "Materials Chemistry for a Sustainable Energy Economy", a new class that he developed. Currently, he is an Honorary Senior Visiting Scholar in the Dept. of Chemistry at Washington University in St. Louis. His awards include eight Sandia awards for research, leadership, and teamwork; a 2014 R&D100 Award (for a novel approach to radiation detection); and Electrochemical Society Fellow. He was also the 2006-2007 President of The Electrochemical Society.

2024 Janet Andersen Award Lecture

Changing Perspectives in Analytical Chemistry

Dr. Ken Brown
John H. and Jeanne M. Jacobson Professor of Chemistry
Hope College

Abstract: This presentation will discuss the emergence and evolution of interdisciplinary research in Analytical Chemistry at Hope College. Many societal problems in science and medicine must be addressed through interdisciplinary research, oftentimes involving Analytical Chemistry. Several areas of research in electrochemistry, environmental justice, and neuroscience will be touched upon in this presentation. The talk will conclude with a detailed look at an iron-based electrochromic system that has been studied in the Brown Lab.

About Dr. Brown: Dr. Kenneth Brown is an analytical chemist at Hope College. His research program has produced 19 papers with 40 undergraduate co-authors in the Journal of Physics and Chemistry Research, the Journal of Electrochemistry, International Journal of Plant Sciences and Analytical Letters among others. His collaborative research with Hope students has focused on electrochemical preparation and characterization of chemically modified electrodes, and connects to and promotes environmental justice. He led a six-year project, funded by the National Science Foundation, which provided summer research experiences for students from the City Colleges of Chicago. He also earned funding from the National Institutes of Health, Howard Hughes Medical Institute, Hope College and the Michigan Space Grant Consortium. In 2024, Dr. Brown received Hope College's Vanderbush-Weller Award for making extraordinary contributions to the lives of students. Ken's students appreciate his unwavering support for their personal development. Dr. Brown also has been named an A. Paul Schaap Fellow in support of his research. Dr. Brown graduated from Oral Roberts University with a Bachelor of Science degree in chemistry. He completed his Ph.D. in chemistry at Oklahoma State University, where he held a NASA Graduate Fellowship.

About the Janet Andersen Award Lecture

Professor Janet Andersen was a beloved faculty member of the Hope College Mathematics Department and served as the Midstates Consortium Director before her life ended tragically in an automobile accident in 2005. As a teacher and scholar, Janet provided creative, high quality learning experiences for her students. She always learned as she was teaching. As Consortium Director, she looked for ways to connect with and support natural science faculty, both new and experienced. To honor Janet's work in her teaching, research and service to the Consortium, the Janet Andersen Lecture Award was established in 2008. Each year, nominees from the Consortium are selected by the Executive Committee to present the Janet Andersen Lecture at the Undergraduate Research Symposia on a topic of his or her expertise.

ORAL SESSION I.A: 10:30 - 11:30 am Room: 201 Moderator: Murphy Brasuel			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
I.A.1	Tatum Goforth	Washington University in St. Louis	Increasing Heterogeneity in In-Silico Metagenomes Resulting in Varying Quality MAGs and Genome Annotations
I.A.2	Daniel Ruskin	Washington University in St. Louis	Mapping Transcription Factor Regulatory Networks in Human Tissues Using Ensemble Learning
I.A.3	Ronan Hanley	Washington University in St. Louis	Signatures of Optimality in Allocation of Cellular Resources to Organelle Number vs. Size
I.A.4	Holly Restad	Washington University in St. Louis	Aβ(1-40) in a Nanoscale Test Tube; LDAO/10MAG Reverse Micelle Encapsulation of Amyloid Beta

ORAL SESSION I.B: 10:30 – 11:30 am Room: 250 Moderator: Paul Fischer			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
I.B.1	Shabab Kabir	Grinnell College	Longevity of Xenon Trapping in Ruthenium-Supported Silica Nanocages
I.B.2	Andrew Valentini	Carthage College	Non-Completely Positive Dynamics as a Probe of Entanglement in Quantum Circuits
I.B.3	Whitney Short	Washington University in St. Louis	Quantum Algorithms for Modeling Open Quantum Systems at Temperature with the Bloch-Redfield Equation
I.B.4	LeClaire Torgelson	Grinnell College	Variable Temperature Diffusion in Mixed Anion Electrolytes for Lithium and Lithium-Ion Batteries

SESSION I.C: 10:30 – 11:30 am Room: 301 Moderator: Katherine Harris			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
I.C.1	Archer Li	Washington University in St. Louis	Comparing Q-Learning Algorithms in Maze Learning Across Environmental Complexity
I.C.2	Thomas Li	Washington University in St. Louis	Dynamic Lambda Estimation for Efficient Market Making in High-Frequency Trading
I.C.3	Eric Seo	Beloit College	Optimized White Sox Lineup Construction with Machine Learning Ensemble Model and Monte-Carlo Game Simulation
I.C.4	Hannah Kim	Grinnell College	Generalization of the Social Golfer Problem

WiFi Access: WUSTL-Guest-2.0

Oral Session II Schedule

SESSION II.D: 2:15 – 3:15 pm Room: 201 Moderator: Michael Gerten			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
II.D.1	Matthew Blake	St. Olaf College	Alternating Harmonic Series Grouped by Fibonacci and Triangular Numbers
II.D.2	Sydney Mayer	Washington University in St. Louis	Investigating Spiral Knots
II.D.3	Vu Anh Le	Beloit College	Assessing the Site Closure Time Frame for Soil and Groundwater Contaminated Sites

SESSION II.E: 2:15 – 3:15 pm Room: 250 Moderator: Graham Sazama			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
II.E.1	Iman Deanparvar and Frannie Drake	Carthage College	Synthesis of Amino Acid Surfactants to Examine Antimicrobial Properties
II.E.2	Yuji Xue	Macalester College	Investigating Odorant Receptor Enantiomer Discrimination Mechanism
II.E.3	Clare O'Brien	Grinnell College	Sourcing Gun Flints: Archaeological Chemistry

SESSION II.F: 2:15 – 3:15 pm Room: 301 Moderator: Kristen Burson			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
II.F.1	Chloe Isabella Tsang	University of Chicago	Design and Implementation of an Inductively Coupled Plasma Source
II.F.2	Cassidy Metzger	Washington University in St Louis	A Survey of eROSITA-WISE Selected TeV-emitting BL Lac Objects
II.F.3	Bishop Carl	Hope College	Next-Generation Neutron Detector: Study of Position Resolution
II.F.4	Erin Coleman	Gustavus Adolphus College	Investigating Methods of Fitting Quasinormal-Modes in Numerical-Relativity Ringdown Signals

WiFi Access: WUSTL-Guest-2.0

Poster Session P1

9:00 a.m. – 10:15 noon Room: Rettner Gallery & 3rd floor hallway			
Poster #	**Presenter Name**	**Institution**	**Title of Presentation**
P1.01	Owen Bonnett, Sikiel Graves & Jordan Wheeler	Carthage College	Validating an Ullage Detection Technique for Liquid Propellant Tanks
P1.02	Teagan Steineke and Justin Wheeler	Carthage College	Towards the Response of Discontinuous Linear Systems to Stationary Random Excitation for Ullage Detection
P1.03	Juliana Alvarez and Skylar Farr	Carthage College	Microgravity Ullage Formation and Trapping Using Phased Array Acoustic Excitation
P1.04	Hope Weeda	Hope College	Effect of Energy-Dependent Proton Irradiation on Thin-Film YBa2Cu3O7−δ Superconductor
P1.05	Liam Gallagher	St. Olaf College	A New Definition of Outsplitting on K-Graphs Preserving Morita Equivalence
P1.07	Mackenzie Amann	St. Olaf College	Looped Zero Forcing on the Set of Graph Loopings
P1.08	Mina Mandegar and Helin Wang	Lawrence University	Generic Rigidity in 3-Space
P1.09	Liu Scott and Daisy Nguyen	Lawrence University	Generic Rigidity of Frames in 3-Space
P1.10	Ian Clawson	Grinnell College	Du Val Singularities in Virtual Reality
P1.11	Samantha Hall, Jianna Pollack and Eloise McSurdy	Grinnell College	Modeling Elephant Movement with Random Walk Models
P1.12	Rohan Avula and Sean Wang	Washington University in St. Louis	Improving the Dynamic Sensitivity of Plasmonically Enhanced Immunoassays
P1.13	Ronard Pabi	Gustavus Adolphus College	Optimum Echo Time for Improved Contrast in T2-Weighted Fast Spin Echo Prostate MRI
P1.14	Oliver Beland and Trenten Chalik	Colorado College	Optimizing Chromatographic Purification Strategies for the Synthesis of a *Pseudomonas aeruginosa* Prodrug
P1.15	Jasmine Najari	Washington University in St. Louis	Engineering a Live Bacterial Therapeutic with a Two-Input Kill Switch for Treating Phenylketonuria
P1.16	Sabrina Schneider	Washington University in St. Louis	Interrogating the Role of the Human Gut Virome in the Development of *Clostridioides difficile* Infection
P1.17	Caroline Cramer	Washington University in St. Louis	Interplay between Anion-Receptor and Anion-Solvent Interactions in Halide Receptor Complexes Characterized with Ultrafast Infrared Spectroscopies

P1.18	James Bradley	Macalester College	Rotational Structure of Electronic States of VF in the Near IR Region
P1.19	Dongting Li	Washington University in St. Louis	Understanding the Nature of Csp3-H···O Hydrogen Bonding Interactions in Rigid Organic Cages
P1.20	Douglas Thibodeaux	Washington University in St. Louis	Nested Sampling for Noble Gas Adsorption on Graphene
P1.21	Charles Fioriglio	Washington University in St. Louis	Studying the Vibrational Dependence of Photoelectron Angular Distributions

Poster Session P2

12:45 p.m. – 2:00 p.m. Room: Rettner Gallery & 3rd floor hallway			
Poster #	**Presenter Name**	**Institution**	**Title of Presentation**
P2.01	Sabra Catalano	Colorado College	Pass the Gas: Mapping Galactic Gas Outflow from the LMC
P2.02	Patrick Loos	Colorado College	Barhopping Between Galaxies: The Azimuthal Variations of Barred Galaxie
P2.03	Emma Weissling	Hope College	Beta-Decay Feeding Intensity Distribution of 93Rb
P2.04	Lucas Peterson	Carthage College	Utilizing Machine Learning to Massively Speed Up Simulations of Terrestrial Gamma-ray Flashes
P2.05	Dawson Gaynor	Carthage College	Orientation Sensing for Electric Field Sensors for Thunderstorms
P2.06	Arya Menk	Gustavus Adolphus College	Investigating the Great September Comet of 1882
P2.07	Meera Dasgupta	University of Chicago	Evaluating GPU-Enabled E3SM/SCREAM Global Climate Model Simulations: A Hurricane Irma Case Study
P2.08	Frances Monroe and Miranda Vizoso-Marino	Gustavus Adolphus College	Environmental Controls on Stromatolite Morphology in the Ordovician Prairie Du Chien Group
P2.09	Kaisa Whittaker and Kendall Wiggins	Gustavus Adolphus College	Human Conflict and Soil Erosion, Environmental and Land Use Change Within the Early Modern Period
P2.10	Teague Merrill	Hope College	Determining Mitochondrial DNA Binding of Proteins Involved in One Carbon Metabolism
P2.11	Samantha Anderson	Gustavus Adolphus College	Exosome Mediated Decay of mRNA of *Saccharomyces cerevisiae*
P2.12	Hannah Parish	University of Chicago	Evolved TadA-assisted m6Am Sequencing in mRNA Caps
P2.13	Amanda Gary	Washington University in St. Louis	Engineering Potentiated Hsp104:NBD1 Variants to Enhance Disaggregase Activity and Substrate Specificity for Alpha-Synuclein Misfolding Rescue
P2.14	Pierce Hoenigman	University of Chicago	Elucidating the Protein Design Space Using Variational Autoencoders
P2.15	Maryam Adebisi	University of Chicago	High-Throughput Fluorescent Protein Tagging of the *Saccharomyces cerevisiae* Genome Using Automated Liquid Handling
P2.16	Gabrielle Shirley and Isaac Stewart	Hope College	Biodegradable Metallopolymers: Kinetic Studies on the Polymerization of Cyclic Carbonate Monomers with Pendant Metallocenes

P2.17	Eva McKinney and Pauline Werks	St. Olaf College	Electrochemical Aerobic Epoxidation of Alkenes Using a Biomimetic Manganese Porphyrin
P2.18	Sarah Solomon	Macalester College	1,2,3 Triazole Synthesis and Reaction
P2.19	Precious Odejimi	Knox College	Computational Analysis of Model Iron Cyclooctadiene Catalysts Supported by Substituted Bis(imino)acenaphthene Ligands
P2.20	Matthew Oberlander	St. Olaf College	Characterization of N2P2 Cobalt Complexes and their Potential as Alternative Catalysts
P2.21	Claire Scott	Hope College	LC/UV-vis and LC/MS/MS to Study the Retinal Carotenoids of Songbirds as a Factor of Habitat and Diet
P2.22	Catherine Rosenbaum and Oliver Beland	Colorado College	Green Solvent Optimization for Solid-Phase Peptide Synthesis of a *Pseudomonas aeruginosa* Prodrug

Poster Session P3

3:30 p.m. – 4:45 p.m. Room: Rettner Gallery & 3rd floor hallway			
Poster #	**Presenter Name**	**Institution**	**Title of Presentation**
P3.01	John Levering	Hope College	Formation of Surface Specific Nanocomposites Due to Sliding
P3.02	Ethan De Koker	Hope College	Impact of Molecular Functionality on Chemical Reactions Activated by Friction
P3.03	Emily Xu	University of Chicago	Differentiating Healthy Aging, Early, and Intermediate Age-Related Macular Degeneration via Retinal Thickness in Optical Coherence Tomography - ALSTAR2 Baseline
P3.04	Mariela López González & Yiwei Yan	Grinnell College	Bulk Refractive Index Sensitivity of LSPR Sensors on Substrate
P3.05	Alexandria Roy	Grinnell College	Xenon Trapping on Diverse Metal-Supported Silica Nanocages
P3.06	Ridham Dholaria and Santosh Pant	Knox College	Virtual Clicker: A Cost-Effective Alternative to IClicker Systems
P3.07	Oscar Reza Bautista	Macalester College	Exploring ViT and CNN-LSTM Architectures to Aid Indoor Robot Localization and Navigation
P3.08	Sydney Ohr	Macalester College	Significance Threshold Estimation for Admixture Mapping (STEAM), an R Package
P3.09	Kyle Suelflow	Macalester College	Age Heaping in Probability Surveys in Sub-Saharan Africa: Frequency and Consequences for Mortality Estimation
P3.10	Phoenix Jarosz	Washington University in St. Louis	City-Scale Species Distribution Modeling Through Aerial Imagery
P3.11	Naysha Jain	Knox College	Music Genre Classification through Discriminative Machine Learning Techniques
P3.12	Frances Hilliard	Knox College	Synthesis and Analysis of Disubstituted Stilbenes: Development of an Advanced Synthesis Lab Course
P3.13	Dana Hicks	Macalester College	Potassium Salts of Diphenylbis (3,5-dimethylpyrazolyl) borates and their Reactions with Iron(II) Chloride
P3.14	Kiely Thompson	Knox College	Synthesis of Phosphonate Estolides from Castor Oil
P3.15	Itzel Vega Juarez	Lawrence University	Synthesis and Characterization of NDI-TTM2•

P3.16	Lindsay Therese Monkam	Macalester College	Cycloaddition of Maleimides for Novel Asymmetric Aromatic Diimides
P3.17	Navraj Singh	Lawrence University	Novel Gold Catalyzed Synthesis of 1H-Isochromenes
P3.18	Jack Lubbs	Knox College	Substitution of Copper(II) Carboxylate Caprolactam Adducts without Donor Solvents
P3.19	Guanchen Zhu	University of Chicago	Asymmetric Total Synthesis of Bipolarolide A-B

Abstracts for all Sessions

Physical Sciences, Mathematics and Computer Science

MCMS Undergraduate Research Symposium, Washington University in St. Louis
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Presenter(s): Adebisi, Maryam
School: University of Chicago
Session: P2.15
Title: High-Throughput Fluorescent Protein Tagging of the *Saccharomyces cerevisiae* Genome Using Automated Liquid Handling
Co-Author(s): Alexander Puch, Eric Zhai, Rohanna Hasselkus
Advisor(s): David Pincus

Abstract: Fluorescent protein fusions are powerful tools commonly used in molecular biology to track protein localization, monitor exogenous protein expression, and investigate genomic modifications. These studies are particularly efficient in the model organism Saccharomyces cerevisiae (budding yeast), due to its robust homologous recombination system which allows for precise insertion of tags into the genome. However, despite the ease of genetic manipulation in yeast, there does not yet exist a scalable, reliable, and optimized high-throughput protocol for genome-wide fluorescent tagging. Current methods often require extensive manual labor which limits the scope and speed of experiments. Here, we present a high-throughput, automated method for fluorescently tagging genes in S. cerevisiae using PCR-mediated transformation. By utilizing the Tecan Liquid Handling Robot, we streamline key experimental steps such as PCR setup, transformation, and colony selection, enabling rapid, parallel processing of multiple samples. This significantly reduces manual intervention and minimizes human error. The high-throughput nature of our protocol opens new avenues for investigating cellular processes in yeast at an unprecedented scale, facilitating new discoveries in functional genomics, protein dynamics, and systems biology.

Presenter(s): Alvarez, Juliana and Farr, Skylar
School: Carthage College
Session: P1.03
Title: Microgravity Ullage Formation and Trapping Using Phased Array Acoustic Excitation
Co-Author(s): Skylar Farr, Reece Greenwald, Semaje Farmer
Advisor(s): Dr. Kevin Crosby

Abstract: Microgravity Ullage Trapping (MUT) is a companion experiment to the Carthage Space Sciences Laboratory program's Microgravity Ullage Detection (MUD) experiment. The Objective of MUT is to form and trap ullage bubbles in earth-storable propellants for use in venting ullage gas during propellant transfer operations. The future of long-term sustainable space exploration is difficult to achieve without a way to refuel a spacecraft while in-flight. In microgravity, propellant adheres to the inner walls of the propellant tank due to adhesion with the tank wall. A gas bubble, or ullage, remains in the center of the tank. The uncontrolled location of the ullage presents a challenge to propellant transfer during refueling. Specifically, the ullage must be located at a vent port in a client tank during the refueling process. MUT implements ultrasonic acoustic excitation of dissolved pressurant gasses in the propellant to both grow bubbles from micron-scale to cm-scale and to drive bubbles along the acoustic pressure field gradient. To establish proof of

concept of Bjerknes Forces which are forces that move and grow bubbles with acoustic excitation we will be conducting a small-scale experiment. This will utilize a single ultrasonic transducer and a waveform generator.

Presenter(s): Amann, Mackenzie
School: St. Olaf College
Session: P1.07
Title: Looped Zero Forcing on the Set of Graph Loopings
Co-Author(s): Hawea Derauf, Brianna Gorny, Adam Berliner
Advisor(s): Adam Berliner

Abstract: The minimum rank problem, also known as the maximum nullity problem, focuses on finding the minimum possible rank (over R) of all the matrices in the collection of symmetric matrices whose underlying zero-nonzero structure is described by a particular (possibly looped) graph G. Zero forcing is a method of coloring vertices in a graph in order to learn more about the maximum nullity of the graph. Stemming from prior research involving simple graphs, this poster explores how loops change the zero forcing number and the overall range of zero forcing numbers for a specific graph. Zero forcing numbers for basic graphs such as paths and complete graphs are discussed, and we solve the zero forcing problem for all looped complete bipartite graphs.

Presenter(s): Anderson, Samantha
School: Gustavus Adolphus College
Session: P2.11
Title: Exosome Mediated Decay of mRNA of *Saccharomyces cerevisiae*
Co-Author(s):
Advisor(s): Jeff Dahlseid

Abstract: The structure and functions of a cell are dictated by information contained within the biological molecule DNA. To utilize the information contained within DNA, the cell synthesizes a molecule of messenger RNA (or mRNA), which contains a copy of the information found in DNA in a highly similar molecular form. mRNA is used to inform the construction of protein, which can perform a variety of functions within the cell. The amount of protein can be regulated through the degradation of the mRNA that encodes it. My research focuses on mRNA degradation in Saccharomyces cerevisiae, specifically through the pathway of Exosome Mediated Decay. The exosome is a multiprotein complex found within the cell that degrades mRNA through a pathway distinct from the default pathway, so its activity may be additive and used to regulate protein levels. The mRNA for an unknown regulator of the CTF13 gene is predicted to be one of the targets of Exosome Mediated Decay. The purpose of this research is to identify this mRNA and determine the features that are responsible for its recognition by the exosome. I am using two different approaches in my research, one utilizing biochemical techniques, and the other using genetics.

Presenter(s): Avula, Rohan and Wang, Sean
School: Washington University in St. Louis
Session: P1.12
Title: Improving the Dynamic Sensitivity of Plasmonically Enhanced Immunoassays
Co-Author(s): Yixuan Wang, Rohit Gupta, Ananya Benegal, Michael D. Vahey, Srikanth Singamaneni

Advisor(s): Srikanth Singamaneni

Abstract: For improving the ultrasensitive and quantitative detection of low-abundance biomarkers on standard immunoassays, many groups have attempted to improve the sensitivity of the fluorophore or nanoparticle used. In addition to better reporter elements, a rarely discussed, yet crucial limitation to sensitivity is analyte bulkiness and binding orientation. We explore two inexpensive and effective improvements: high-avidity synthetic antibodies and cyclic draining and replenishing technology (CDR) to improve the dynamic sensitivity of plasmonic-fluor based lateral flow assays (p-LFA) and immunosorbent assays (p-FLISA). Our high-avidity synthetic antibody improves the sensitivity of p-LFAs by optimizing analyte binding orientation through multivalent binding afforded by conjugating LCB1 affibodies (antibody mimetic miniproteins) to bovine serum albumin (BSA). Due to the size of Plasmonic Fluor, steric hindrance effects limit antigen binding and sensitivity. CDR uses periodic rotation of the assay to promote binding efficiency of the PF reporter element for both the sandwich assay and competitive ELISA. Overall, we report significant improvements in sensitivity in immunoassays through the novel application of various techniques.

Presenter(s): Beland, Oliver and Chalik, Trenten
School: Colorado College
Session: P1.14
Title: Optimizing Chromatographic Purification Strategies for the Synthesis of a *Pseudomonas aeruginosa* Prodrug
Co-Author(s): Cate Rosenbaum, Ty Kruger, Amy Dounay
Advisor(s): Amy Dounay

Abstract: *Pseudomonas aeruginosa*, a bacterium common in cystic fibrosis patients, forms biofilms that contribute to drug-resistance and complicate treatment. Two carbohydrate binding proteins, LecA and LecB, were identified within the biofilm and can be used for targeted drug delivery. A prodrug combining the antibiotic compound 4-fluoro-L-phenylalanine (4-FPhe) with a LecA probe was proposed, aiming to minimize cytotoxicity while maintaining antimicrobial properties. A key component of this prodrug is a pentapeptide containing 4-FPhe. Purifying the pentapeptide from incomplete intermediates has proven difficult. Intermediates accumulated during solid phase peptide synthesis (SPPS) exhibited similar chromatographic properties to the desired peptide. Therefore, isolation through medium pressure liquid chromatography (MPLC) was challenging. Significant progress towards the purification of the pentapeptide was made through adapting an ultra-performance liquid chromatography (UPLC) method to an MPLC procedure. Furthermore, N-acetyl capping was explored to enhance alternative purification strategies. Ongoing optimization efforts are focused on improving the MPLC purification method and N-acetylation to isolate sufficient quantities of pentapeptide for coupling to the LecA sugar probe.

Presenter(s): Beland, Oliver and Rosenbaum, Catherine
School: Colorado College
Session: P2.22
Title: Green Solvent Optimization for Solid-Phase Peptide Synthesis of a *Pseudomonas aeruginosa* Prodrug
Co-Author(s): Trenten Chalik, Ty Kruger, Amy Dounay
Advisor(s): Amy Dounay

Abstract: *Pseudomonas aeruginosa* is an opportunistic pathogen that, due to a high degree of antibiotic resistance, commonly affects immunocompromised individuals – particularly those with cystic fibrosis. A prodrug containing 4-fluoro-L-phenylalanine (4-FPhe) designed to target the LecA and LecB enzymes present in *P. aeruginosa* biofilms, minimizes cytotoxicity and maximizes antimicrobial activity. A key component of this prodrug is a pentapeptide containing 4-FPhe. Solid phase peptide synthesis (SPPS) commonly utilizes dichloromethane (DCM) for resin loading, and N,N-dimethylformamide (DMF) for acylation. Both solvents are acutely toxic and hazardous. SPPS optimization focused on identifying green, cost-effective, and accessible solvent alternatives. Resin loading was completed with Acetonitrile/ethyl acetate (EtOAc) (1:1). Previous acylation reactions in EtOAc were inefficient and produced minimal yield. Six binary solvent mixtures with similar polarities to DMF were assessed. Dimethyl sulfoxide (DMSO)/2-methyltetrahydrofuran (2-Me-THF) (3:7) and DMSO/1,3 – dioxolane (DOL) (4:6) significantly improved reaction times and yields.

Presenter(s): Blake, Matthew
School: St. Olaf College
Session: II.D.1
Title: Alternating Harmonic Series Grouped by Fibonacci and Triangular Numbers
Co-Author(s):
Advisor(s): Sooie-Hoe Loke, Dominic Klyve

Abstract: In 2011, Chen and Kennedy explored reordering the Alternating Harmonic Series, rearranging the terms into blocks whose sizes are given by the Fibonacci numbers. In this work, we modify their approach in two ways: we replace the Fibonacci numbers with the triangular numbers, and we remove Chen and Kennedy's parity restriction on the sign of each term; we thus create three new series. We analyze convergence and boundedness of all four series, finding that while the original diverges but is bounded, two of the new series converge, while the final series diverges without bound. Next, inspired by the Riemann zeta function, we consider a new family of series by exponentiating every blocked term by a positive power . We analyze properties of these generalized series, including convergence and boundedness. Finally, we use a generalized linear model to find functions which calculate partial sums for various exponents , and use these formulas to hypothesize asymptotic behavior of these generalized sums.

Presenter(s): Bonnett, Owen; Graves, Sikiel; Wheeler, Jordan
School: Carthage College
Session: P1.01
Title: Validating an Ullage Detection Technique for Liquid Propellant Tanks
Co-Author(s): Justin Wheeler, Sikiel Graves, Jordan Wheeler, Teagan Steineke
Advisor(s): Kevin Crosby

Abstract: The Microgravity Ullage Detection (MUD) experiment is an element of a larger effort to address ullage venting during in-space refueling operations. Carthage College, in collaboration with the Johnson Space Center Power and Propulsion division, is developing technologies to locate the ullage bubble in a propellant tank and to facilitate the venting of ullage gas during refueling. The MUD payload has two primary technical objectives: (1) demonstrate that, under gravity, a liquid-vapor interface can be detected non-invasively using external acoustic patch sensors mounted on the tank, and (2) demonstrate that, under microgravity, changes in the thickness of the adhered liquid layer can be measured non-invasively during a tank drain using

external acoustic patch sensors mounted on the tank. Ullage detection is accomplished by exploiting the fact that the sensor output is sensitive to the local stiffness and damping of the tank wall. By calculating the Root Mean Square of the sensor at a given location, liquid presence and interface velocity at the location of the sensor can be inferred, thus identifying the location and geometry of the ullage. Under gravity, the location of fluid interface has been determined with resolution of < 1% of the full-tank volume for settled liquids.

Presenter(s): Bradley, James
School: Macalester College
Session: P1.18
Title: Rotational Structure of Electronic States of VF in the Near IR Region
Co-Author(s): Grant Luce, Thomas Varberg
Advisor(s): Thomas Varberg

Abstract: A new E5Δ–X5Δ transition of gas-phase vanadium fluoride (VF) at 789 nm has been analyzed and its case (a) rotational constant determined for the first time by recording its laser excitation spectrum. Five main electronic subbands (Ω = 0–0 to 4–4) were observed, with the satellite (ΔΩ = ±1) subbands too weak to be identified. Ram, Bernath and Davis (J. Chem. Phys. 2002, 116, 7035–7039, DOI: 10.1063/1.1464831) previously analyzed several vibrational bands of a different 5Δ–X5Δ transition in the near infrared but were unable to identify an Ω = 0–0 subband due to severe spectral congestion. Our spectrum displays Λ-doubled R and P branches for each subband, but no Q branches due to their low predicted intensity in a parallel (ΔΩ = 0) transition. The data were fitted using an effective Hamiltonian written in a Hund's case (a) basis. The fitted value of ground state rotational constant is B = 0.38097(13) cm–1, which yields a bond length of R0 = 1.788(3) Å.

Presenter(s): Carl, Bishop
School: Hope College
Session: II.F.3
Title: Next-Generation Neutron Detector: Study of Position Resolution
Co-Author(s): Belen Monteagudo, Paul DeYoung, Thomas Baumann
Advisor(s): Paul DeYoung , Belen Monteagudo

Abstract: The MoNA Collaboration is designing the Next-Generation Neutron Detector (NGn) to improve the position resolution of neutron detection in invariant-mass spectroscopy experiments. More accurate position resolution of neutrons improves the overall reconstructed decay energy of unbound states, which leads to better understanding of exotic nuclei near the neutron dripline. A small scale prototype of the future NGn was fabricated out of a scintillating plastic and a modular array of Silicon Photomultipliers (SiPMs) with DAQ supported by a Front-End Readout System (FERS). This prototype allows for testing of different configurations of the experimental setup with minimal effort. Configurations include different combinations of the following: wrapping of the scintillating plastic, presence of optical coupling, and different spacing between the SiPMs. Position resolution is being studied through a multi-regression decision forest algorithm based on simulation. The currently predicted position resolution using the machine learning algorithm is ~1 cm. To validate simulation, a new calibration method was developed which exclusively uses the internal pulser of the FERS with no need of external equipment. Preliminary results of these ongoing tests will be presented.

Presenter(s): Catalano, Sabra
School: Colorado College
Session: P2.01
Title: Pass the Gas: Mapping Galactic Gas Outflow from the LMC
Co-Author(s): Anders Ripley
Advisor(s): Dhanesh Krishnarao

Abstract: Galactic winds are crucial to understand their host galaxies in terms of star formation rates, stellar masses, metal content, spatial distribution, and other observable properties. However, due to the complexity that they can be driven by multiple sources, it is hard to resolve and observationally identify their components and their sources. The Large Magellanic Cloud (LMC), a nearby galaxy of the Milky Way, serves as an ideal target to analyze different galactic wind properties due to its proximity, face-on geometry, and abundance of multi-wavelength data. We used archival data from the ULYSSES survey, focusing on the Cosmic Origins Spectrograph onboard the Hubble Space Telescope to measure absorption features of O I (neutral oxygen) and Si II (singly ionized silicone) to trace the cool gas in winds emerging from the LMC. We normalized the absorption continuum and employed VoigtFit to measure absorption line velocities, column densities, and line widths. Based on out fit results, we provide preliminary maps of the column density and weighted average velocity of outflowing gas in comparison to the disk of the LMC. This study is part of a larger HST Legacy Archival program (HST-AR 16602; PI Barger) to map the LMC wind in fine detail across several ion tracers and gas phases.

Presenter(s): Chalik, Trenten and Beland, Oliver
School: Colorado College
Session: P1.14
Title: Optimizing Chromatographic Purification Strategies for the Synthesis of a *Pseudomonas aeruginosa* Prodrug
Co-Author(s): Cate Rosenbaum, Ty Kruger, Amy Dounay
Advisor(s): Amy Dounay

Abstract: *Pseudomonas aeruginosa*, a bacterium common in cystic fibrosis patients, forms biofilms that contribute to drug-resistance and complicate treatment. Two carbohydrate binding proteins, LecA and LecB, were identified within the biofilm and can be used for targeted drug delivery. A prodrug combining the antibiotic compound 4-fluoro-L-phenylalanine (4-FPhe) with a LecA probe was proposed, aiming to minimize cytotoxicity while maintaining antimicrobial properties. A key component of this prodrug is a pentapeptide containing 4-FPhe. Purifying the pentapeptide from incomplete intermediates has proven difficult. Intermediates accumulated during solid phase peptide synthesis (SPPS) exhibited similar chromatographic properties to the desired peptide. Therefore, isolation through medium pressure liquid chromatography (MPLC) was challenging. Significant progress towards the purification of the pentapeptide was made through adapting an ultra-performance liquid chromatography (UPLC) method to an MPLC procedure. Furthermore, N-acetyl capping was explored to enhance alternative purification strategies. Ongoing optimization efforts are focused on improving the MPLC purification method and N-acetylation to isolate sufficient quantities of pentapeptide for coupling to the LecA sugar probe.

Presenter(s): Clawson, Ian
School: Grinnell College
Session: P1.10

Title: Du Val Singularities in Virtual Reality
Co-Author(s): Shibam Mukhopadhyay
Advisor(s): Christopher French

Abstract: The focus of this research was to develop a new way of learning about du Val singularities or singular points through the use of virtual reality (VR). Singularities are points on a surface that are not smooth, and we cannot define a tangent plane at these points. One way mathematicians studied singularities was through the creation of models, and particularly in the 19th century these models were made of plaster. In studying singularities, the ability to manipulate the object, such as rotating or resizing, is helpful in getting a better perspective to what is occurring mathematically. While possible in plaster models, VR provides a better environment to accomplish this task. Our VR experience challenges the user to identify singularities on cubic and quartic surfaces, as well as classify these singular points by ADE classification, a method of sorting singularities into equivalence classes. Through this experience we believe the user gets a more intuitive feel for what a du Val singularity is and what type of surfaces have these singularities.

Presenter(s): Coleman, Erin
School: Gustavus Adolphus College
Session: II.F.4
Title: Investigating Methods of Fitting Quasinormal-Modes in Numerical-Relativity Ringdown Signals
Co-Author(s): Eliot Finch
Advisor(s): Eliot Finch

Abstract: The ringdown of a black hole merger can be decomposed into quasinormal modes (QNMs), and it has been suggested that the subset of QNMs known as overtones can contribute significantly. This work aims to measure the contribution of each overtone to the ringdown via fits to numerical-relativity waveforms, which has implications for analysis of ringdown signals and tests of general relativity (GR). We employ both least-squares and Bayesian fitting methods, and use several different metrics to determine each overtone's importance. The first metric used is the earliest time at which a model with N overtones is a good fit (i.e., the ringdown start time). Each additional overtone allows an earlier fit, however the change in start time decreases with N. The second metric introduces deviations from the GR frequency of each overtone. We found that the effect of deviations decreases rapidly with overtone index n. This implies it becomes harder to perform tests of GR with each additional overtone. The third metric is the stability of mode amplitudes between fits with different ringdown start times. It is known that least-squares fits are not optimal for studying amplitudes, and here we perform a Bayesian analysis for more robust results.

Presenter(s): Cramer, Caroline
School: Washington University in St. Louis
Session: P1.17
Title: Interplay between Anion-Receptor and Anion-Solvent Interactions in Halide Receptor Complexes Characterized with Ultrafast Infrared Spectroscopies
Co-Author(s): Jessika L. S. Dean, Joseph A. Fournier
Advisor(s): Joseph A. Fournier

Abstract: The competition between host-guest binding and solvent interactions is a crucial factor

in determining the binding affinities and selectivity of molecular receptor species. The development of molecular-level descriptions of solute-solvent interactions remains an experimental challenge. We investigate the halide receptor meso Octamethylcalix[4]pyrrole (OMCP) complexed with either chloride or bromide anions in both dichloromethane (DCM) and chloroform (trichloromethane, TCM) solvent using ultrafast infrared transient absorption and 2D IR spectroscopies. OMCP·Br– complexes in both solvents display slower vibrational relaxation dynamics of the OMCP pyrrole NH stretches, consistent with weaker H bonding interactions with OMCP compared to chloride. Further, OMCP·Br– complexes show nearly static spectral diffusion dynamics compared to OMCP·Cl–, indicating larger structural fluctuations occur within chloride complexes. Importantly, distinct differences in the vibrational spectra and dynamics are observed between DCM and TCM solutions. The data are consistent with more perturbative solvent effects in TCM compared to DCM, despite DCM's larger dielectric constant and smaller reported OMCB·X– binding affinities, which are attributed to the presence of weak H bond interactions between halides and TCM, in addition to competing interactions from the bulky tetrabutylammonium countercation. The data provide important experimental benchmarks for quantifying the role of solvent and countercation interactions in anion host-guest complexes.

Presenter(s): Dasgupta, Meera
School: University of Chicago
Session: P2.07
Title: Evaluating GPU-Enabled E3SM/SCREAM Global Climate Model Simulations: A Hurricane Irma Case Study
Co-Author(s): Gökhan Sever, Brandi Gamelin, Dimitrios Fytanidis, Vishwas Rao, Mustafa Altinakar, Peter Perry
Advisor(s): Brandi Gamelin

Abstract: Hurricane Irma was a Category 5 Atlantic hurricane that made landfall in South Florida on September 10th, 2017. At the time, it was considered the strongest hurricane observed on the open Atlantic Ocean and caused $77.16 billion in damages. Climate models have long been used to simulate hurricanes, such as Irma, to forecast these outcomes and better understand their behavior over time. The Energy Exascale Earth System Model (E3SM) project has progressed in optimizing these models to work on exascale machines. The completion of the Simple Cloud Resolving E3SM Atmosphere Model (SCREAMv1), which is capable of running on GPU-enabled exascale machines such as Aurora and Frontier, began addressing the decadal challenge of running E3SM using GPU resources. This presentation will describe a computational evaluation of the current phase of the E3SM model project in development using a GPU-enabled machine, Polaris, for a case study of Hurricane Irma. The evaluation of the model is expected to contribute to greater insights into the effect of initialization start dates on simulation results and set expectations for how higher-resolution model data might impact the analysis of natural disasters, especially on island nations.

Presenter(s): De Koker, Ethan
School: Hope College
Session: P3.02
Title: Impact of Molecular Functionality on Chemical Reactions Activated by Friction
Co-Author(s): Ashton Wolford
Advisor(s): Meagan Elinski

Abstract: Produced energy is largely rejected due to losses attributed to friction. Lubrication and

anti-wear additives which promote wear reduction and decrease overall friction have been the main solutions to conserve energy. One mechanism that allows for energy conservation is the usage of additives that undergo the formation of anti-wear films on surfaces by mechanical forces. However, the current commercial additive is a metal-organic compound containing sulfur, rendering it environmentally harmful and subject to increasing regulations limiting its use. An alternate solution focuses on tribochemical reactions that can readily polymerize molecules, forming carbon-based anti-wear films, but there is a limited understanding of these films. This work focused on different molecules and how differences in molecular structure can affect tribopolymerization. Cyclic and linear molecules that vary the positioning of alkene, alcohol, and oxygen functional groups were added to a polyalphaolefin oil (PAO4) and used as lubricants in sliding processes subjected to steel-on-steel interactions. The surfaces were analyzed with Raman spectroscopy and scanning electron microscopy post-sliding to examine the presence of polymer formation on the surface. Further work understanding molecules that can readily polymerize to form anti-wear films under mechanical stress can present possible tribological solutions to conserving energy.

Presenter(s): Deanparvar, Iman and Drake, Frannie
School: Carthage College
Session: II.E.1
Title: Synthesis of Amino Acid Surfactants to Examine Antimicrobial Properties
Co-Author(s): Cole Hanson, Aileen Szczepanski, David Brownholland
Advisor(s): David Brownholland

Abstract: Bacteria are evolving to develop antibiotic resistance at ever increasing rates, necessitating the need for new antimicrobial agents. Amino acid surfactants have generated interest as possible antimicrobial agents due to their biodegradability and ability to be synthesized from renewable feedstocks. An ester-linked leucine-based surfactant was previously synthesized by our group and found to exhibit antimicrobial properties. The synthetic procedure of this molecule is currently being optimized to improve purification and yield. However, the ester linkage between the amino acid headgroup to the hydrophobic tail is susceptible to hydrolysis. In order to address this limitation, the surfactant was redesigned to use a more stable amide linkage, rather than an ester. We report the progress of the synthesis of this amide-linked surfactant. The resulting surfactant will be analyzed for its antimicrobial properties and the results of these assays will be used to help design new generations of antimicrobial surfactants.

Presenter(s): Dholaria, Ridham and Pant, Santosh
School: Knox College
Session: P3.06
Title: Virtual Clicker: A Cost-Effective Alternative to IClicker Systems
Co-Author(s): Santosh Pant
Advisor(s): Michael Gerten

Abstract: Student response systems like iClicker, widely used in classrooms, often impose financial burdens on students by requiring the purchase of hardware. To address this issue, our project, Virtual Clicker, proposes a cost-effective, cloud-based platform that enhances classroom engagement and eliminates the need for dedicated devices. The platform allows instructors to create customizable question types, such as multiple-choice, true/false, and open-ended formats, while providing students with real-time feedback. It securely stores all data in the cloud, allowing easy access for both students and instructors. Additionally, an analytics dashboard provides

instructors with real-time insights into student performance and participation. Designed for both mobile and desktop devices, the platform is highly accessible and user-friendly, making it a seamless alternative to traditional iClicker systems. By leveraging cloud technologies, Virtual Clicker reduces costs, encourages active participation, and improves data management, aligning with institutional goals of enhancing student services and incorporating technology to improve educational outcomes. Our ten-week development plan involves system design, frontend and backend development, testing, and deployment, with the anticipated outcome of providing a flexible, affordable solution for classroom engagement. This project contributes to reshaping traditional learning environments by fostering interactive, collaborative experiences and empowering instructors to better monitor and support student progress.

Presenter(s): Drake, Frannie and Deanparvar, Iman
School: Carthage College
Session: II.E.1
Title: Synthesis of Amino Acid Surfactants to Examine Antimicrobial Properties
Co-Author(s): Cole Hanson, Iman Deanparvar, Frannie Drake, Aileen Szczepanski, David Brownholland
Advisor(s): David Brownholland

Abstract: Bacteria are evolving to develop antibiotic resistance at ever increasing rates, necessitating the need for new antimicrobial agents. Amino acid surfactants have generated interest as possible antimicrobial agents due to their biodegradability and ability to be synthesized from renewable feedstocks. An ester-linked leucine-based surfactant was previously synthesized by our group and found to exhibit antimicrobial properties. The synthetic procedure of this molecule is currently being optimized to improve purification and yield. However, the ester linkage between the amino acid headgroup to the hydrophobic tail is susceptible to hydrolysis. In order to address this limitation, the surfactant was redesigned to use a more stable amide linkage, rather than an ester. We report the progress of the synthesis of this amide-linked surfactant. The resulting surfactant will be analyzed for its antimicrobial properties and the results of these assays will be used to help design new generations of antimicrobial surfactants.

Presenter(s): Farr, Skylar and Alvarez, Juliana
School: Carthage College
Session: P1.03
Title: Microgravity Ullage Formation and Trapping Using Phased Array Acoustic Excitation
Co-Author(s): Kevin Crosby, Juliana Alvarez, Reece Greenwald, Semaje Farmer
Advisor(s): Kevin Crosby

Abstract: Microgravity Ullage Trapping (MUT) is a companion experiment to the Carthage Space Sciences Laboratory program's Microgravity Ullage Detection (MUD) experiment. The Objective of MUT is to form and trap ullage bubbles in earth-storable propellants for use in venting ullage gas during propellant transfer operations. The future of long-term sustainable space exploration is difficult to achieve without a way to refuel a spacecraft while in-flight. In microgravity, propellant adheres to the inner walls of the propellant tank due to adhesion with the tank wall. A gas bubble, or ullage, remains in the center of the tank. The uncontrolled location of the ullage presents a challenge to propellant transfer during refueling. Specifically, the ullage must be located at a vent port in a client tank during the refueling process. MUT implements ultrasonic acoustic excitation of dissolved pressurant gasses in the propellant to both grow bubbles from micron-scale to cm-scale and to drive bubbles along the acoustic pressure field gradient. To establish proof of

concept of Bjerknes Forces which are forces that move and grow bubbles with acoustic excitation we will be conducting a small-scale experiment. This will utilize a single ultrasonic transducer and a waveform generator.

Presenter(s): Fioriglio, Charles
School: Washington University in St. Louis
Session: P1.21
Title: Studying the Vibrational Dependence of Photoelectron Angular Distributions
Co-Author(s):
Advisor(s): Richard Mabbs

Abstract: Photoelectron angular distributions (PADs) carry information about the nature of molecular orbitals. Good theoretical models for photodetatchment are crucial in accurate treatment of electron molecule interactions such as energy transfer, capture, and scattering. PADs, characterized by the anisotropy parameter (ß), have typically been treated assuming a sole dependance on the shape of the parent orbital. However, experimental data for O2– photodetatchment (O2– --> O2 + e–) shows that ß also depends strongly on which vibrational level of the neutral is accessed. Varying bond lengths have been treated computationally using a united atom model and approximating the parent molecular orbital as an atomic orbital. However, this offers little physical insight as the model only accounts for spatial extent of the parent orbital and does not consider vibrational channel. A molecular approach within the Franck-Condon approximation fails to replicate the experimental trends, and so it has been hypothesized that to recover the experimental trends, separation of the electronic and nuclear motion is inappropriate. In a rigorous testing of this claim, ß values were calculated using ab initio determined parent orbitals over a range of bond lengths to account for vibronic coupling, producing some surprising results.

Presenter(s): Gallagher, Liam
School: St. Olaf College
Session: P1.05
Title: A New Definition of Outsplitting on K-Graphs Preserving Morita Equivalence
Co-Author(s): Mackenzie Amann, Liam Gallagher, Rachael Norton
Advisor(s): Rachael Norton

Abstract: We introduce a novel graph move, LiMaR-Split, which is applicable to higher rank graphs. This move allows us to transform a given higher rank graph into a new higher rank graph. We demonstrate that the original graph’s underlying structure and that of the graph obtained through LiMaR-Split are equivalent up to Morita equivalence.

Presenter(s): Gary, Amanda
School: Washington University in St. Louis
Session: P2.13
Title: Engineering Potentiated Hsp104:NBD1 Variants to Enhance Disaggregase Activity and Substrate Specificity for Alpha-Synuclein Misfolding Rescue
Co-Author(s): Meredith Jackrel, Karlie Miller, Kira Jones, Allan Wang
Advisor(s): Meredith Jackrel

Abstract: Protein misfolding is a key driver of many neurodegenerative diseases, including Parkinson’s Disease (PD). PD is associated with the accumulation of alpha-synuclein, a

lipid-binding protein that can clump in Lewy bodies and become toxic. Wild-type Hsp104 is a AAA+ protein disaggregase from yeast that has weak disaggregase activity on substrates involved in neurodegenerative diseases, such as alpha-synuclein. However, Hsp104 variants can be engineered to improve this activity. Our work focuses on testing the alpha-synuclein-specific disaggregase activity of Hsp104 variants with mutations in the nucleotide-binding domain 1 (NBD1) of Hsp104. Using a yeast-based toxicity screen, we selected key variants from a deep mutational scan of NBD1. Three NBD1 variants have been identified that appear to specifically rescue toxicity of alpha-synuclein in a yeast model. These variants display temperature sensitivity and are being tested in thermotolerance assays to investigate their toxicity and ability to promote recovery from protein misfolding at elevated temperatures. Microscopy will be completed to analyze the variant's disaggregation activity. Eventually, selected variants will be purified and evaluated in mammalian cells. The outcomes of this project could contribute to research on Hsp104 as a potential therapeutic for neurodegenerative diseases with alpha-synuclein-specific disaggregase activity and toxicity rescue.

Presenter(s): Gaynor, Dawson
School: Carthage College
Session: P2.05
Title: Orientation Sensing for Electric Field Sensors for Thunderstorms
Advisor(s): Brant Carlson

Abstract: Electric fields in thunderstorms are hard to study, as current balloon-borne probes are large and slow, causing problems by limiting the picture of electric field geometry and biasing electric field results. These problems can be solved by launching multiple freefalling probes. Freefalling probes need to spin to measure the electric fields, leading to uncertain orientation. This project aims to develop effective orientation sensing methods for freefalling probes. Two sensors were designed for orientation sensing: a vibration sensor and a wire coil sensor. The vibration sensor, sensitive to gravity, produces a sinusoidal voltage signal that can be used to determine both the frequency of rotation and the rotational position of the probe. The coil sensor, sensitive to Earth's magnetic field, outputs a similar sinusoid that, when used in conjunction with the vibration sensor, can determine a compass heading. Initial testing shows that the vibration sensor works, while further work needs to be done for the coil. Future work will entail working on integrating these sensors with one another and, eventually, with a full free-falling probe.

Presenter(s): Goforth, Tatum
School: Washington University in St. Louis
Session: I.A.1
Title: Increasing Heterogeneity in In-Silico Metagenomes Resulting in Varying Quality MAGs and Genome Annotations
Advisor(s): Gautam Dantas, Wesley Agee

Abstract: The quality of genome assembly from metagenome-assembled genomes (MAGs) is critical for understanding microbial communities. In this study, we explored the assembly quality of individual species' MAGs using a long-read MAG assembly pipeline. We assembled MAGs from varying numbers of microbial species and evaluated their quality by comparing the assembled genomes to the reference genomes. This comparison allowed for an assessment of genome completeness, contamination, and quality of the assembled MAGs. Our findings provide insights into the effectiveness of long-read MAG generation and offer guidelines for optimizing assembly pipelines to achieve higher-quality genomes, particularly

for complex metagenomic samples. These results contribute to the broader field of microbial genomics and the development of computational pipelines for assessing and annotating genomes assembled from mixed-species samples.

Presenter(s): Graves, Sikiel; Bonnett, Owen; Wheeler, Jordan
School: Carthage College
Session: P1.01
Title: Validating an Ullage Detection Technique for Liquid Propellant Tanks
Co-Author(s): Justin Wheeler, Jordan Wheeler, Teagan Steineke, Owen Bonnett
Advisor(s): Kevin Crosby

Abstract: The Microgravity Ullage Detection (MUD) experiment is an element of a larger effort to address ullage venting during in-space refueling operations. Carthage College, in collaboration with the Johnson Space Center Power and Propulsion division, is developing technologies to locate the ullage bubble in a propellant tank and to facilitate the venting of ullage gas during refueling. The MUD payload has two primary technical objectives: (1) demonstrate that, under gravity, a liquid-vapor interface can be detected non-invasively using external acoustic patch sensors mounted on the tank, and (2) demonstrate that, under microgravity, changes in the thickness of the adhered liquid layer can be measured non-invasively during a tank drain using external acoustic patch sensors mounted on the tank. Ullage detection is accomplished by exploiting the fact that the sensor output is sensitive to the local stiffness and damping of the tank wall. By calculating the Root Mean Square of the sensor at a given location, liquid presence and interface velocity at the location of the sensor can be inferred, thus identifying the location and geometry of the ullage. Under gravity, the location of fluid interface has been determined with resolution of < 1% of the full-tank volume for settled liquids.

Presenter(s): Hall, Samantha; McSurdy, Eloise; Pollack, Jianna
School: Grinnell College
Session: P1.11
Title: Modeling Elephant Movement with Random Walk Models
Co-Author(s): Eloise McSurdy, Jianna Pollack, Owen Gould
Advisor(s): Pratima Hebbar

Abstract: We conducted an in-depth study of modeling elephant movement using random walks, introducing a memory-driven approach called the Adaptive Movement Model (AMM). While we briefly discuss the theoretical foundations of random walks, our primary emphasis is on their application to understanding the behavioral patterns of elephants in Kruger National Park, South Africa. Our analysis identifies two statistically significant behavioral states — 'Encamped' and 'Exploratory' — which are influenced by environmental factors such as precipitation. Our AMM integrates a range of ecological factors influencing elephant behavior, offering a more nuanced representation of their movement dynamics. It incorporates advanced topics in random walks, such as random environments and dependencies based on both location and time. Our research not only enhances the understanding of elephant behavior but also offers valuable insights for conservation strategies. Ultimately, our findings underscore the potential of memory-driven random walk models in capturing the complexities of animal movement in variable environments.

Presenter(s): Hanley, Ronan
School: Washington University in St. Louis
Session: I.A.3

Title: Signatures of Optimality in Allocation of Cellular Resources to Organelle Number vs. Size
Co-Author(s): Fang Yu, Shixing Wang, Ronan Hanley, Shankar Mukherji
Advisor(s): Shankar Mukherji

Abstract: Among the hallmarks of the eukaryotic cell is its organization into spatially defined subcompartments known as organelles. Organelles provide optimized environments for otherwise incompatible biochemical reactions within the cell. In order to tailor organelle biogenesis to its needs, the cell can regulate the size and number of many of its organelles. This begs the question: what principles dictate how much of the cell's limited resources are devoted to increasing the number versus the size of a given organelle? We propose that cellular resource allocation to organelle number and size is consistent with a simple optimality principle: resources are optimally allocated to organelle number and size growth for de novo synthesized organelles, while organelle numbers and sizes themselves are optimized for fission derived organelles. Our framework makes two predictions: the organelle size to number ratio for de novo versus fission derived organelles should scale with total organelle volume with opposite slopes and that fission-mediated organelle biogenesis can exhibit critical behavior. Employing hyperspectral imaging, we observed both distinct signatures of optimality in mitochondria, Golgi and lipid droplets. This work represents a potential step toward uncovering the general rules that dictate resource allocation during the processes eukaryotic cells use to build their organelles.

Presenter(s): Hicks, Dana
School: Macalester College
Session: P3.13
Title: Potassium Salts of Diphenylbis (3,5-dimethylpyrazolyl) borates and their Reactions with Iron(II) Chloride
Co-Author(s): Paul Fischer, Sandy Goldstein, Victor Young
Advisor(s): Paul Fischer

Abstract: My summer research concerned the synthesis of potassium salts of diphenylbis(3,5-dimethylpyrazolyl)borates, for reactions with iron(II) chloride ($FeCl_2$), based on known phenyltris(3,5-dimethylpyrazolyl)borates previously characterized by the Fischer lab. The later trispyrazolyl borates prefer bidentate coordination to iron(II) metal centers despite possessing three nitrogen atoms eligible to attach to iron. Our new bispyrazoyl borates are intended to coordinate via two nitrogen atoms, and without the presence of unbound nitrogen atoms that could compete with substrates intended to react with the metal. The bispyrazoyl borates were successfully reacted with $FeCl_2$, and the intended complexes, with each bispyrazolyl ligand attached to the metal via two nitrogen atoms, were obtained. Preliminary observations of these complexes indicate that these Fe(II) centers may harbor some electronic unsaturation which could be leveraged for reactions.

Presenter(s): Hilliard, Frances
School: Knox College
Session: P3.12
Title: Synthesis and Analysis of Disubstituted Stilbenes: Development of an Advanced Synthesis Lab Course
Advisor(s): Diana M. Cermak

Abstract: Stilbenes are a group of compounds identifiable by their unique structure: a central

alkene with two aromatic ring substituents, predominantly favoring the trans orientation. Stilbenes are found in nature, including various medicinal plants, peanuts and the skin of grapes. They have also been found to possess a number of beneficial biochemical properties, displaying anti-inflammatory, anti-oxidant, and anti-cancer effects. Stilbenes can be synthesized via a variety of synthetic routes, many of which can incorporate a variety of graduate-level organic laboratory techniques. This research focused on synthesizing para-disubstituted stilbenes with unsymmetric substituents in a way that would teach undergraduates many new advanced lab techniques and characterizing them with advanced NMR techniques. Thus, a two-step process was chosen: an Arbuzov Reaction of a substituted benzyl halide, followed by a Horner-Wadsworth-Emmons (HWE) Condensation with a substituted aldehyde. The viable stilbenes will be implemented in an advanced lab course to familiarize students with graduate level laboratory and analytical techniques, including methods for handling air-sensitive reagents, low-temperature techniques, and NMR spectroscopic methods such as 31P, 19F, DEPT-135, and HSQC NMR spectra. A wide variety of para-disubstituted stilbenes were chosen for each student to synthesize a unique molecule; progress on this project will be presented.

Presenter(s): Hoenigman, Pierce
School: University of Chicago
Session: P2.14
Title: Elucidating the Protein Design Space Using Variational Autoencoders
Advisor(s): Rama Ranganathan

Abstract: Protein design is a long-standing goal of synthetic biology and medicine, but until recently we have lacked sufficient data and computational power. Variational autoencoders are a deep learning architecture which have proven useful in learning the amino acid sequence patterns to generate novel proteins by first compressing large sequences into a low-dimensional latent space. Yet despite their ability to replicate the sequence patterns of protein families, the models are overfit to evolutionary noise and thus are not able to produce diverse proteins. Additionally, the functional properties of the protein are not well separated in the latent space, and therefore using the models for more precise protein engineering is infeasible. Statistical coupling analysis is a method which has shown great utility in disentangling the functional properties of a protein family. This project aims to connect the functional awareness of statistical coupling analysis with the generative capability of variational autoencoders to create a more diverse, interpretable, and controllable protein generative model.

Presenter(s): Iwerks, Pauline
School: St. Olaf College
Session: P2.17
Title: Electrochemical Aerobic Epoxidation of Alkenes Using a Biomimetic Manganese Porphyrin
Co-Author(s): Eva McKinney, Tashani Williams and Sarah Oppenheim
Advisor(s): Anna Brezny

Abstract: Producing various medications and other necessary products such as detergents and pesticides. In nature, molecules called metalloenzymes use energy and oxygen gas to create epoxides. However, in a laboratory setting, it is difficult to directly use oxygen due to its low reactivity. Consequently, scientists depend on traditional methods of epoxidation that utilize hazardous chemicals. Compounds called metalloporphyrins are structurally similar to metalloenzymes allow scientists to catalyze epoxidation reactions safely and efficiently. Our proposed method uses a manganese metalloporphyrin catalyst, oxygen gas, and an electrical

current to produce epoxides. Reaction products were analyzed by H-NMR to identify hydrogens in potential epoxide products based on the symmetry in the structure. Analyses indicate epoxide yields of up to 75%. The use of metalloporphyrins with oxygen creates a safe and efficient way to synthesize epoxides without using harsh chemicals.

Presenter(s): Jain, Naysha
School: Knox College
Session: P3.11
Title: Music Genre Classification through Discriminative Machine Learning Techniques
Advisor(s): Nathalie Haurberg

Abstract: This independent study – conducted over two months – looked into applying various discriminative algorithms on multiple music genres and figured out the best algorithm to do so. We applied multiple discriminative algorithms to classify over 10 music genres based on their acoustic properties. We evaluated algorithms such as Random Forest, Support Vector Machines (SVM), Linear Regression, K-Nearest Neighbors (KNN), and Decision Trees. We developed a Python-based framework to analyze these genres quantitatively, achieving classification accuracy exceeding 70%. The dataset included both personal music samples and publicly available data from Kaggle. Confusion matrices were used for performance comparison across models. In the final phase, we studied the classification of a corpus of punk music using our methods and produced various results.

Presenter(s): Jarosz, Phoenix
School: Washington University in St. Louis
Session: P3.10
Title: City-Scale Species Distribution Modeling Through Aerial Imagery
Co-Author(s): Srikumar Sastry, Adeel Ahmad, Nathan Jacobs
Advisor(s): Nathan Jacobs

Abstract: We present a high-resolution species distribution model (SDM) for the Greater St. Louis area, leveraging deep learning to map species presence by using crowdsourced presence-only species observations and 1-meter resolution aerial imagery. Prior work generates low-resolution range maps, making those models unsuitable for local conservation efforts. Aerial imagery provides fine-grained environmental features that allows the model to learn about the habitat of where species are present. To improve predictive accuracy and explore the significance of absence data, we visually compare two models: a baseline SDM using only presence data and a variant (RS-SDM) that integrates pseudo-absence data by randomly sampling locations and assuming they have no species presence. A visualization method is used to produce range maps of every species in our dataset.

Presenter(s): Kabir, Shabab
School: Grinnell College
Session: I.B.1
Title: Longevity of Xenon Trapping in Ruthenium-Supported Silica Nanocages
Co-Author(s): Erik Genet, Alexandria Roy, Kristen Burson, Jorge Anibal Boscoboinik
Advisor(s): Jorge Anibal Boscoboinik

Abstract: The isolation and purification of noble gases are essential processes applicable to radon abatement, nuclear waste isolation, and anesthetics. However, these processes are

also expensive and energy-intensive, often employing temperatures as low as 4 K. Recent advancements have explored alternative methods, including physically trapping noble gases in metal-supported nanostructures. In this study, we investigate the longevity of xenon trapping in the silica nanocage DodecaPhenyl Polyhedral Oligomeric Silsesquioxane (DP-POSS), which is deposited on a Ru(0001) substrate. A near-monolayer amount of DP-POSS was successfully deposited on Ru(0001) with a Langmuir-Blodgett trough. Subsequent calcination and reduction of DP-POSS to POSS allows for xenon trapping capabilities. Continuously performing X-ray photoelectron spectroscopy (XPS) monitored the stability of xenon trapped in different environments over time. Our results indicate that xenon is lost over time in both ultra-high vacuum and ambient-pressure conditions, but the loss rate is significantly faster in ambient-pressure conditions. Xenon located at interstitial sites is lost first, due to being in a more unstable state than the xenon physically confined in POSS. Our work suggests that DP-POSS depositions on ruthenium substrates could serve as noble gas traps with significant retention times, offering a viable room-temperature alternative to existing noble gas separation technologies.

Presenter(s): Kim, Hannah
School: Grinnell College
Session: I.C.4
Title: Generalization of the Social Golfer Problem
Advisor(s): Collin Nolte

Abstract: This research focuses on generalizing approximate solutions to the Social Golfer problem (SGP), a combinatorial challenge that iteratively assigns subjects to groups subject to the constraint that repeated pairings are minimized. We generalize existing solutions by introducing the ability to specify loss functions which produce a numeric score indicating consistency of a proposed pairing subject to arbitrary constraints. Our presentation illustrates at a high level how we search the space of possible solutions through the use of permutations and mutations, as well as how we instantiate loss functions in this context. We conclude by demonstrating practical use-cases for this type of solution. For example, pedagogical literature suggests that there is value in pairing students according to aptitude, and our proposed generalization of the SGP would allow for instructors to create pairings that minimizes within-group differences based on assessment scores while also reducing the number of repeated pairs.

Presenter(s): Le, Vu Anh
School: Beloit College
Session: II.D.3
Title: Assessing the Site Closure Time Frame for Soil and Groundwater Contaminated Sites
Co-Author(s): Haruko Murakami Wainwright
Advisor(s): Haruko Murakami Wainwright

Abstract: Monitored Natural Attenuation (MNA) is an increasingly recognized remidiation method for its cost-effective and minimally invasive approach to managing soil and groundwater contamination. By extending the PyLEnM machine learning framework, we developed a data-driven model to estimate the time for contaminants like Sr-90 and I-129 to reach regulatory safety standards. The study integrates linear regression, random forest regression, and an ensemble LSTM model to analyze trends in contaminant concentrations, accounting for the site's complex hydrostratigraphic units and geochemical conditions. Preliminary results indicate a

significant downward trend in contaminant levels, with the maximum time to reach safety thresholds being 320 years for Sr-90 and 258 years for I-129 amongst decreasing wells. Our findings highlight the importance of specific hydrological factors, such as total depth and screen zone, in enhancing the predictability and effectiveness of MNA strategies, ensuring long-term groundwater protection. The study scope covers the Savannah River Site (SRS), a Department of Energy-owned Superfund site contaminated with radionuclides that plans to apply MNA.

Presenter(s): Levering, John
School: Hope College
Session: P3.01
Title: Formation of Surface Specific Nanocomposites Due to Sliding
Co-Author(s): Gloria Kozak, Anna Zini
Advisor(s): Meagan B. Elinski

Abstract: The common occurrence of degenerative diseases, such as osteoarthritis, has led to an influx in treatments using nanoparticles as drug-delivery systems. However, there is little knowledge on the fate of nanoparticles when slid against a soft surface such as cartilage. Based on nanoparticle behavior sliding against hard surfaces, a number of outcomes are possible ranging from negative (surface wear), to neutral, to positive (surface protection through nanoparticle compaction). Prior work investigating frictional behavior of nanoparticles sliding against a soft surface observed residual particle debris, but it is still unclear what mechanisms are at play for surface modification. This work implements cartilage-mimicking polyacrylamide (PAM) hydrogels as a model for biological tissue, seeking to answer if nanoparticles are embedded in the hydrogel surface as a result of sliding forces. Different levels of applied axial load were used for macroscale sliding tests in the presence of zirconium dioxide nanoparticles. Post-sliding surfaces were analyzed with Raman spectroscopy and scanning electron microscopy (SEM) to determine if force via sliding drove the formation of nanocomposites. Further work will expand understanding of these types of chemical-mechanical relationships, enabling the in situ formation of nanocomposite materials and broadening the array of disease treatment capabilities.

Presenter(s): Li, Archer
School: Washington University in St. Louis
Session: I.C.1
Title: Comparing Q-Learning Algorithms in Maze Learning Across Environmental Complexity
Co-Author(s): Apoorva Arora, Unmukt Gupta, Adam Kepecs
Advisor(s): Adam Kepecs

Abstract: Achieving a balance between exploration and exploitation is a fundamental challenge in reinforcement learning (RL), particularly in environments with complex dynamics and large state spaces. The exploration-exploitation dilemma revolves around the agent's need to explore uncertain actions to discover potentially better outcomes while also exploiting known actions to maximize immediate rewards. This balance is crucial for learning optimal policies efficiently.
Here, we focus on evaluating different strategies within the Q-learning framework to address this challenge in maze environments of varying complexities. Maze environments, with their structured yet varied layouts, provide an ideal platform for assessing how different exploration algorithms adapt to environments of differing intricacy.
Past research has highlighted that the effectiveness of RL algorithms can vary significantly across different maze complexities. In simpler mazes, agents may benefit from more

straightforward exploration strategies and vice versa.
To address these challenges, we formally modeled state space complexity in our environment for analysis, then systematically compared several Q-learning exploration strategies: ϵ-greedy, Upper Confidence Bound-1 (UCB-1), softmax, and pursuit. Each strategy is evaluated as a function of complexity based on 1) cumulative sum of obtained rewards, 2) convergence speed, 3) robustness and adaptability to changes in the environment, and 4) exploration efficiency.

Presenter(s): Li, Dongting
School: Washington University in St. Louis
Session: P1.19
Title: Understanding the Nature of Csp3-H···O Hydrogen Bonding Interactions in Rigid Organic Cages
Co-Author(s): Fangzhou Li and Javed Pathan
Advisor(s): Chenfeng Ke

Abstract: In our previous work, we reported a tripodal cage molecule with high affinity to perchlorate by the unconventional C_{sp3}-H···O hydrogen bonds. The interaction is formed between the O of the perchlorate and the protons of piperazine moieties, whose direction is restricted by the carbonyl group neighboring it. In this project, we will verify the effect of the C_{sp3}-H···O hydrogen bond by removing carbonyl groups. Due to the absence of carbonyl groups in the new cage molecule, the pre-organized status of the H on piperazine is lost, allowing it to freely rotate. Hence, the binding affinity to the perchlorate ion of the new cage is expected to decrease due to a weaker interaction between the cage and the anion. The synthesis of the cage involves five steps, and each intermediate and final product will be characterized using ^{1}H NMR spectroscopy. The new tripodal cage's affinity to perchlorate ions will be examined by ^{1}H NMR titration experiment.

Presenter(s): Li, Thomas
School: Washington University in St. Louis
Session: I.C.2
Title: Dynamic Lambda Estimation for Efficient Market Making in High-Frequency Trading
Advisor(s): José E. Figueroa-López

Abstract: This research explores the development and application of a predictive model for estimating liquidation costs in high-frequency trading, focusing on the calculation of the price impact parameter, lambda, within a Limit Order Book framework. Building on the strategy which models the market maker's optimal choice in the presence of stochastic liquidity demand, this study introduces a novel approach to dynamically estimate lambda using linear regression on historical limit order book data. Specifically, we compute lambda for both bid and ask sides at the end of each trading day, average these values, and then apply ARIMA modeling to predict future lambdas. The predictive model is validated over a series of 50 trading days, with initial estimates based on the first 20 days and subsequent predictions refined using actual daily lambda calculations. This research provides insights into optimizing liquidation strategies and managing end-of-day inventory, contributing to more efficient market-making practices.

Presenter(s): Loos, Patrick
School: Colorado College

Session: P2.02
Title: Barhopping Between Galaxies: The Azimuthal Variations of Barred Galaxie
Co-Author(s): Aliana Istanbullu
Advisor(s): Dhanesh Krishnarao

Abstract: Galactic bars, prominent structures in many spiral galaxies, significantly contribute to the evolution of galaxies by funneling gas from the outer regions to the core, which can fuel star formation and influence galactic structure and chemical composition. While bars may increase star formation rates and trigger active galactic nuclei (AGN) in some cases, their overall effect of star formation and metallicity remains debated, with differing results depending on galaxy type, bar strength, and length. Some studies suggest bars are more common in redder, passive spirals, while others show mixed findings on their impact on stellar population and galaxy morphology. However, azimuthal variations of galaxy parameters and their relationship to bars is not well known. With a sample of SDSS-IV MaNGA galaxies, we analyze how different parameters vary with azimuth in a range of barred galaxies. The goal of our research is to compare the azimuthal variations we found with predictions from galaxy simulations. Our research also provides insight into the correlation between galaxy properties and dark gaps, which are regions in barred galaxies where there is a significant decrease in light along the bar's minor axis compared to its major axis, resulting in a seemingly darker region.

Presenter(s): López González, Mariela and Yan, Yiwei
School: Grinnell College
Session: P3.04
Title: Bulk Refractive Index Sensitivity of LSPR Sensors on Substrate
Co-Author(s): Yiwei Yan, Keisuke Hasegawa
Advisor(s): Keisuke Hasegawa

Abstract: Localized surface plasmon resonance (LSPR) biosensors are a popular label-free detection method for detecting biological molecules. These sensors rely on the optical properties of metal nanoparticles (NPs) and the collective oscillation of their free electrons upon incident waves. LSPR sensors include in-suspension and on-substrate, where the latter has not been extensively studied. Building on the understanding of substrate-nanoparticle interactions is important for the design of on-substrate sensors. We theoretically investigate the bulk refractive index (RI) sensitivity of immobilized gold NPs of various geometries (square, disk, hexagon, cuboid, cylinder, triangle, and rod). Using MNPBEM, a MATLAB toolbox, we verify that the effect of the substrate on the RI sensitivity is dependent on the NP shape. The smallest decrease in the bulk RI sensitivity is seen for nanorod and nanocylinder, whereas plate-like shapes show a significant decrease in the sensitivity once immobilized. We combine effective medium and quasistatic theory to derive an analytical expression for predicting the sensitivity. The expression presents the best accuracy for rod and cylinder shapes. The low-impact substrate effect and high theoretical accuracy make these NP geometries suitable for sensor design.

Presenter(s): Lubbs, Jack
School: Knox College
Session: P3.18
Title: Substitution of Copper(II) Carboxylate Caprolactam Adducts without Donor Solvents
Co-Author(s): Thomas Clayton, Sahana Giri
Advisor(s): Thomas Clayton

Abstract: Copper(II) carboxylate dimers have been shown to exhibit liquid crystalline properties, with varying phases and melting point depending on the length and structure of the carboxylate ligands. A substitution scheme has been previously established wherein carboxylates of varying size and structure can be introduced to create mono and di-substituted dimers in toluene with a donor solvent (THF, acetonitrile). It has also been shown that these dimers form caprolactam adducts on the introduction of caprolactam, resulting in lower melting points and birefringence. This work examines the substitution reactions of Copper(II) hexanoate caprolactam adducts without the presence of a donor solvent. With varying amounts of caprolactam, the substitution of a caprolactam adduct was still observed. Infrared spectroscopy (FT-IR), polarized optical microscopy (POM), differential scanning calorimetry (DSC) and elemental analysis were used to characterize these products. IR analysis demonstrated an outsized amide peak when the exchange was done with 6 equivalents of caprolactam. In addition, further X-ray crystallographic analysis of this product after recrystallization in toluene resulted in a new polymorph of unsubstituted hexanoate caprolactam adduct.

Presenter(s): Mandegar, Mina and Wang, Helin
School: Lawrence University
Session: P1.08
Title: Generic Rigidity in 3-Space
Co-Author(s): Helin Wang, Daisy Nguyen, Liu Scott
Advisor(s): Alexander Michael Heaton

Abstract: We study the combinatorial rigidity of bar-joint frameworks in 3-space. A graph embedded in space is called "rigid" when all other embeddings preserving the edge-lengths are rigid motions of Euclidean space, meaning translations, rotations, or reflections. A graph is called "flexible" otherwise, since a one-parameter family of embeddings which do not arise from rigid motions may be visualized as a physically realizable structure deforming and losing its shape. In particular, we study the X-replacement and double-V replacement conjectures. These graph operations are conjectured to preserve rigidity. We verified the non-existence of counterexamples on graphs with less than 15 vertices computationally. Finally, we also provided explicit proofs of the "reverse" 2-extension theorem which makes the X and double-V replacements so important.

Presenter(s): Mayer, Sydney
School: Washington University in St. Louis
Session: II.D.2
Title: Investigating Spiral Knots
Co-Author(s): Ashish Das, Luke Moyar, Faisal Quraishi
Advisor(s): Sarah Blackwell, Ryan Stees

Abstract: Torus knots are an important family of knots about which much is understood; invariants of torus knots often exhibit nice formulae, making them convenient and fundamental building blocks for examples in knot theory. Spiral knots are a braid-theoretic generalization of torus knots, but not much is known about this broader family of knots. We give a general formula for the Alexander polynomial of spiral knots, and from this we derive several properties of spiral knots, including a simple formula for their genus. Additionally, we investigate the consequences these results have on classification questions.

Presenter(s): McKinney, Eva
School: St. Olaf College

Session: P2.17
Title: Electrochemical Aerobic Epoxidation of Alkenes Using a Biomimetic Manganese Porphyrin
Co-Author(s): Pauline Iwerks, Tashani Williams and Sarah Oppenheim
Advisor(s): Anna Brezny

Abstract: Producing various medications and other necessary products such as detergents and pesticides. In nature, molecules called metalloenzymes use energy and oxygen gas to create epoxides. However, in a laboratory setting, it is difficult to directly use oxygen due to its low reactivity. Consequently, scientists depend on traditional methods of epoxidation that utilize hazardous chemicals. Compounds called metalloporphyrins are structurally similar to metalloenzymes allow scientists to catalyze epoxidation reactions safely and efficiently. Our proposed method uses a manganese metalloporphyrin catalyst, oxygen gas, and an electrical current to produce epoxides. Reaction products were analyzed by H-NMR to identify hydrogens in potential epoxide products based on the symmetry in the structure. Analyses indicate epoxide yields of up to 75%. The use of metalloporphyrins with oxygen creates a safe and efficient way to synthesize epoxides without using harsh chemicals.

Presenter(s): McSurdy, Eloise; Hall, Samanth; Pollack, Jianna
School: Grinnell College
Session: P1.11
Title: Modeling Elephant Movement with Random Walk Models
Co-Author(s): Jianna Pollack, Owen Gould
Advisor(s): Pratima Hebbar

Abstract: We conducted an in-depth study of modeling elephant movement using random walks, introducing a memory-driven approach called the Adaptive Movement Model (AMM). While we briefly discuss the theoretical foundations of random walks, our primary emphasis is on their application to understanding the behavioral patterns of elephants in Kruger National Park, South Africa. Our analysis identifies two statistically significant behavioral states — 'Encamped' and 'Exploratory' — which are influenced by environmental factors such as precipitation. Our AMM integrates a range of ecological factors influencing elephant behavior, offering a more nuanced representation of their movement dynamics. It incorporates advanced topics in random walks, such as random environments and dependencies based on both location and time. Our research not only enhances the understanding of elephant behavior but also offers valuable insights for conservation strategies. Ultimately, our findings underscore the potential of memory-driven random walk models in capturing the complexities of animal movement in variable environments.

Presenter(s): Menk, Arya
School: Gustavus Adolphus College
Session: P2.06
Title: Investigating the Great September Comet of 1882
Co-Author(s): Qicheng Zhang
Advisor(s): Qicheng Zhang

Abstract: The Great September Comet of 1882 was the brightest known member of the Kreutz family, the only known group of sungrazing comets. We modeled the coma dust surrounding the comet's nucleus to find its physical radius using past observations of the comet between the Earth and the Sun. The model is based on reports of the comet's observed angular diameters and forward scattering appearance created when the incoming and diffracted sunlight are in the

same direction. To account for the reported color of the comet, the average dust size produced needed to be no larger than 1 μm in diameter. The calculated dust production rate of 3.8e7 +/- 1.7e7 kg/s and the derived estimate that 4.2[+1.1,-1.0]% of the sunlight reaching the comet was used to sublimate water yielded a comet size of 17.4[+7.3,-3.3] km in radius. Unlike daily visible Kreutz objects, the Great Comet likely resembled the original progenitor, containing a large fraction of the total mass of the family.

Presenter(s): Merrill, Teague
School: Hope College
Session: P2.10
Title: Determining Mitochondrial DNA Binding of Proteins Involved in One Carbon Metabolism
Co-Author(s): Amanda Lopykinski, Kristin Dittenhafer-Reed
Advisor(s): Kristin Dittenhafer-Reed

Abstract: Mitochondria have their own DNA (mitochondrial DNA, mtDNA) that carries the genetic instructions for some of the proteins required to produce ATP. We are interested in understanding the regulation of the expression of mtDNA, as disruptions in this process are connected with mitochondrial dysfunction leading to human disease. Previous literature determined that thirty-seven proteins are associated with mtDNA (Han et al., 2017), including three proteins involved in one-carbon metabolism: ALDH1L2, SHMT2, and MTHFD1L. Our main question is whether the interaction between one-carbon metabolism proteins and mtDNA controls mitochondrial gene expression and/or mitochondrial DNA maintenance. Our focus is whether one-carbon proteins of interest directly bind to mtDNA, and if so, where they bind in the genome. We employed an in vitro mtDNA binding assay to determine mtDNA binding interactions, which was complemented and quantified by fluorescence polarization and electrophoretic mobility shift assay. We identified a direct interaction between SHMT2 and mtDNA and a potential direct interaction between ALDH1L2 and mtDNA. We also explored whether mtDNA interactions may be mediated through protein-protein interactions and found that SHMT2 potentially binds directly with mitochondrial single-stranded binding protein.

Presenter(s): Metzger, Cassidy
School: Washington University in St. Louis
Session: II.F.2
Title: A Survey of eROSITA-WISE Selected TeV-emitting BL Lac Objects
Co-Author(s): Andrea Gokus, Manel Errando
Advisor(s): Manel Errando

Abstract: The mechanisms of particle acceleration within the relativistic jets produced by active galactic nuclei (AGN) are largely unknown. This is due, in large part, to our limited detection capabilities. While BL Lacertae (BL Lac) objects are the most numerous class of AGN capable of producing extremely high energy gamma rays, only 56 BL Lacs are confirmed to have this capability. We develop a procedure to select extremely energetic BL Lacs based on infrared (IR) and X-ray observations. We combine the eROSITA Main catalog and the WISE ALLSKY catalog to retrieve 158 candidates. We find that 66 of our candidates are confirmed as BL Lac objects in the ROMA-BZCAT catalog. Additionally, 119 of our sources have been proposed as high-synchrotron peaked BL Lac candidates in the 3HSP catalog. We offer a selection of 30 previously unidentified candidates for BL Lacs capable of producing extremely high energy gamma rays. This survey provides an updated target list of candidates for future gamma ray observations.

Presenter(s): Monkam, Lindsay Therese
School: Macalester College
Session: P3.16
Title: Cycloaddition of Maleimides for Novel Asymmetric Aromatic Diimides
Advisor(s): Professort Dennis Cao

Abstract: This research project focuses on diversifying the maleimide R group to synthesize asymmetric aromatic diimides. Our primary objectives are to create a variety of these compounds and investigate how different R groups impact the final product properties. Through this work, the Cao lab aims to better understand structure-property relationships in asymmetric aromatic diimides, potentially paving the way for new materials with specific characteristics.

Presenter(s): Monroe, Frances and Vizoso-Marino, Miranda
School: Gustavus Adolphus College
Session: P2.08
Title: Environmental Controls on Stromatolite Morphology in the Ordovician Prairie Du Chien Group
Co-Author(s): Miranda Vizoso-Marino
Advisor(s): Miranda Vizoso-Marino

Abstract: Stromatolites are organo-sedimentary structures that grow on carbonate platforms. Stromatolite form, at both macro and meso scale is sensitive to changes in the environment. However, the specific ways that environmental factors shape stromatolite morphology remain largely unknown. The stromatolites of the Ordovician Prairie du Chien Group are well-exposed in Minnesota and Wisconsin, and their patterns and changes in both mesostructure and macrostructure may record environmental change in ancient oceans. Multiple field sites in both Minnesota and Wisconsin were visited to investigate stromatolite morphological variability. To investigate the causes of mesostructure change, individual laminae of stromatolites from the Prairie du Chien Group were traced, revealing that the introduction of sand to a stromatolite disturbs stromatolite growth, causing lower inheritance. At the macroscale level, we observed that stromatolites in the upper half of the Prairie du Chien Group are characterized by a transition from small domal layered stromatolites to large, flat-laminated forms. This pattern probably records a shoaling upwards sequence. However, the lower half of the Prairie du Chien Group does not exhibit that same morphological pattern. This difference in macroscale pattern raises a question: what environmental differences separate the lower and upper parts of the Prairie du Chien Group?

Presenter(s): Najari, Jasmine
School: Washington University in St. Louis
Session: P1.15
Title: Engineering a Live Bacterial Therapeutic with a Two-Input Kill Switch for Treating Phenylketonuria
Co-Author(s): Esse M Evbuomwan, Sakshi Khanna, Austin Rottinghaus, Aura Ferreiro, Chenggang Xi, Blake Butler, Jasmine Najari, Matthew D Amrofell, Tae Seok Moon, Gautam Dantas
Advisor(s): Gautam Dantas

Abstract: Phenylketonuria is a genetic disease characterized by the inability to metabolize

phenylalanine, which can result in neurotoxicity and cause neurological deficits, along with emotional and cognitive problems. The standard treatment for PKU is persuading patients to follow a protein-restricted diet, which can be extremely challenging for patients. To provide an alternative treatment plan to strict low-protein dieting, we engineered *Escherichia coli* to express genes encoding Phe-metabilizing enzymes. We included a kill switch within the genome of our engineered *E. coli* expressing Phe-metabolizing enzymes. Upon activation, the chemical and temperature sensitive kill switch triggers pathways that lead to cell death. This allows our strains to self terminate outside the host (30°C) or in response to a chemical compound (aTc). By engineering *E.coli* with both Phe-expressing enzyme capacity and a kill switch, we hypothesize that it is possible to create a next-generation, safe therapeutic for PKU that can be controlled through modulating chemical and temperature input to ensure biocontainment.
To test this hypothesis, we have engineered *E. coli* strains expressing PAL2, and a single input kill switch independently and together in vitro. To test the reliability of the single-input kill switches, we utilized an aTc-induction assay to isolate the loss of function strains at 30°C. PAL2 does not possess TetR resistance cassette, which is why it dies in the presence of aTc. To ensure that the kill switch is not interfering with PAL2 expression, we have utilized a phenylalanine assay to observe whether the degradation of phenylalanine is occurring when expected.

Presenter(s): Nguyen, Daisy; Scott, Liu
School: Lawrence University
Session: P1.09
Title: Generic Rigidity of Frames in 3-Space
Co-Author(s): Helin Wang, Mina Mandegar, Liu Scott
Advisor(s): Alexander Michael Heaton

Abstract: We study the combinatorial rigidity of bar-joint frameworks in 3-space. A graph embedded in space is called "rigid" when all other embeddings preserving the edge-lengths are rigid motions of Euclidean space, meaning translations, rotations, or reflections. A graph is called "flexible" otherwise, since a one-parameter family of embeddings which do not arise from rigid motions may be visualized as a physically realizable structure deforming and losing its shape. In particular, we study the X-replacement and double-V replacement conjectures. These graph operations are conjectured to preserve rigidity. We verified the non-existence of counterexamples on graphs with less than 15 vertices computationally. Finally, we also provided explicit proofs of the "reverse" 2-extension theorem which makes the X and double-V replacements so important.

Presenter(s): O'Brien, Clare
School: Grinnell College
Session: II.E.4
Title: Sourcing Gun Flints: Archaeological Chemistry
Advisor(s): Lee Sharpe

Abstract: Gunflints played a crucial role in firearm ignition during the 18th and 19th centuries. The ability to more confidently differentiate between native manufacture and acquisition from European sources will enhance our understanding of trade patterns and military technology during this period. We are utilizing laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) and principal component analysis (PCA) to chemically source gunflints found in Nepal.

Presenter(s): Oberlander, Matthew
School: St. Olaf College
Session: P2.20
Title: Characterization of N2P2 Cobalt Complexes and their Potential as Alternative Catalysts
Advisor(s): Elodie E Marlier

Abstract: The most commonly used catalysts in industry today employ expensive, environmentally unsustainable transition metals such as rhodium, palladium, iridium, and platinum. Efforts are being made to use safer, more cost-effective first-row transition metals including cobalt, nickel, and zinc for catalytic applications. β-diketiminate (BDI) commonly serves as a ligand scaffold for organometallic catalysts. In this work synthetic variations to BDI are made to create a binding pocket for metals to insert. This poster will explore of a variety of Cobalt (II) metalated BDI ligands utilizing N2P2 binding pockets, and their reduced Cobalt (I) counterparts. The variation for each compound is a result of methyl, dimethyl, or methoxy substituents on the phenyl linkers of the BDI backbone. Characterization through UV-Visible spectroscopy, NMR spectroscopy, and crystallographic data are given to highlight the successful synthesis of each species, analyze the geometry surrounding the metal center, and determine redox properties of each compound. Future work will determine the reactivity of these compounds as catalytic species.

Presenter(s): Odejimi, Precious
School: Knox College
Session: P2.19
Title: Computational Analysis of Model Iron Cyclooctadiene Catalysts Supported by Substituted Bis(imino)acenaphthene Ligands
Advisor(s): Helen M. Hoyt

Abstract: Reduced iron catalyst (dppBIAN)Fe(toluene) (dpp = 2,6-diisopropylphenyl; BIAN = bis(imino)acenaphthene) promotes the hydrosilylation of 1-hexene with phenylsilane in nearly quantitative yield. Precatalyst dppBIANFeBr2 provided similar results upon in situ activation with a reducing agent. However, less sterically protected ArBIANFeBr2 precatalysts provided low-to-modest yields under similar conditions. To understand the theoretical impact of ligand variation on the spin state of the iron's center, a series of less sterically hindered ArBIANFe(cyclooctadiene) complexes were studied computationally. Density Functional theory (DFT) calculations were performed at the B3LYP level of theory, and the method included an empirical relativistic correction (ZORA). Geometry optimization, numerical frequency computation, and Mössbauer isomer shift calculations were performed. All catalysts studied were predicted to have an electronic structure of a high spin iron(I) center antiferromagnetically coupled to the monoreduced ArBIAN ligand. A narrow range of Mössbauer isomer shifts was found for the series, suggesting the isolated catalysts may perform better in catalysis than precatalysts activated in situ. Interestingly, the isomer shift trend for the active catalysts correlates with precatalyst hydrosilylation yields. Computed isomer shifts will be used to determine optimal candidates for experimental analysis in hydrosilylation reactions, particularly toward the reaction of more highly substituted alkenes.

Presenter(s): Ohr, Sydney
School: Macalester College
Session: P3.08

Title: Significance Threshold Estimation for Admixture Mapping (STEAM), an R Package
Co-Author(s): Katelyn McClure, Kelsey Grinde
Advisor(s): Kelsey Grinde

Abstract: Admixture mapping is important for identifying disease genes, especially in populations with mixed ancestry. This summer, we worked on improving an R package, called STEAM, that finds a genome-wide significance threshold that can be used in admixture mapping. Our process started with reviewing how other researchers were utilizing STEAM in their own research projects, and then using this understanding to improve and debug the code. We also prioritized enhancing the usability of the STEAM package with new features and updated documentation in addition to making efforts to increase STEAM's visibility as an R package.

Presenter(s): Pabi, Ronard
School: Gustavus Adolphus College
Session: P1.13
Title: Optimum Echo Time for Improved Contrast in T2-Weighted Fast Spin Echo Prostate MRI
Co-Author(s): Stephen J. Riederer, Eric A. Borisch
Advisor(s): Stephen J. Riederer

Abstract: Prostate cancer is the second most common cancer in men in the United States, with 1 in 8 men diagnosed in their lifetime and 1 in 44 dying from the disease. Early detection and effective treatment are critical for improving patient outcomes. Magnetic Resonance Imaging (MRI), particularly T2-weighted MRI, plays a pivotal role in identifying cancerous lesions in the prostate. However, scan times for T2-weighted MRI can take several minutes, as seen at Mayo Clinic in Rochester, which can be uncomfortable for patients and reduce efficiency for radiologists. This project explores a newly developed sequence for T2-weighted MRI that reduces scan times but initially suffered from poor contrast. Through analysis of phantom and patient scans, we investigated the impact of the MRI parameter, Echo Time (TE), on image contrast. We identified an optimal TE that significantly improved image quality, enabling the sequence to deliver faster scans without compromising diagnostic accuracy. This optimized sequence reduced scan time by approximately 22% while maintaining comparable contrast, thus offering a more efficient method for detecting prostate cancer. The sequence is currently being tested on patients at the clinic, demonstrating its potential to reduce the effects of patient motion on images and enhance clinical workflow as well as patient comfort.

Presenter(s): Pant, Santosh and Dholaria, Ridham
School: Knox College
Session: P3.06
Title: Virtual Clicker: A Cost-Effective Alternative to IClicker Systems
Co-Author(s): Ridham Dholaria
Advisor(s): Michael Gerten

Abstract: Student response systems like iClicker, widely used in classrooms, often impose financial burdens on students by requiring the purchase of hardware. To address this issue, our project, Virtual Clicker, proposes a cost-effective, cloud-based platform that enhances classroom engagement and eliminates the need for dedicated devices. The platform allows instructors to create customizable question types, such as multiple-choice, true/false, and open-ended formats, while providing students with real-time feedback. It securely stores all data in the cloud, allowing easy access for both students and instructors. Additionally, an analytics dashboard provides

instructors with real-time insights into student performance and participation. Designed for both mobile and desktop devices, the platform is highly accessible and user-friendly, making it a seamless alternative to traditional iClicker systems. By leveraging cloud technologies, Virtual Clicker reduces costs, encourages active participation, and improves data management, aligning with institutional goals of enhancing student services and incorporating technology to improve educational outcomes. Our ten-week development plan involves system design, frontend and backend development, testing, and deployment, with the anticipated outcome of providing a flexible, affordable solution for classroom engagement. This project contributes to reshaping traditional learning environments by fostering interactive, collaborative experiences and empowering instructors to better monitor and support student progress.

Presenter(s): Parish, Hannah
School: University of Chicago
Session: P2.12
Title: Evolved TadA-assisted m6Am Sequencing in mRNA Caps
Co-Author(s): Yuan Wu
Advisor(s): Weixin Tang

Abstract: N6,2'-O-dimethyladenosine (m6Am), an RNA modification appearing in the caps of mRNA, serves a number of roles in regulation of gene expression. However, due to an inability to precisely sequence for this modification, studies regarding the role of m6Am have been inconclusive and a more detailed understanding of its mechanisms and functions continues to elude researchers. Previous attempts at mapping and quantifying this modification in the mammalian transcriptome have used FTO, an N6-methyladenosine (m6A) demethylase which prefers m6Am to m6A but does not effectively demethylate all m6Am sites, or antibody sequencing which does not differentiate between m6A and m6Am. Here, we present a new approach to quantifying the percentage of m6Am appearing in the caps of mRNA. Using a method for mapping and quantifying mRNA caps in the mammalian transcriptome in conjunction with evolved TadA-assisted m6A sequencing (eTAM-seq), a method to detect N6-methyladenosine by adenosine deamination, we develop and optimize a protocol to accurately and precisely quantify the m6Am modification in mRNA caps. We additionally explore this method's potential to sequence 5' UTR m6A and m6Am concurrently, which would allow for further elucidation of the functions of both mRNA modifications.

Presenter(s): Peterson, Lucas
School: Carthage College
Session: P2.04
Title: Utilizing Machine Learning to Massively Speed Up Simulations of Terrestrial Gamma-ray Flashes
Advisor(s): Brant Carlson

Abstract: Terrestrial Gamma Ray Flashes (TGFs) are millisecond-long emissions of gamma rays from thunderclouds typically observed by satellites. Photons observed by satellites are subject to scattering and absorption as they escape the atmosphere, so satellite data is often interpreted with the aid of simulation. Such simulations are often slow, especially for sources deep in the atmosphere, due to the high likelihood of absorption. To speed up these simulations, we train a Conditional Generative Adversarial Network (cGAN) to reproduce distributions of photons at satellite altitude resulting from sources with energies from 0.1-10 MeV and incidence angles of 0-90 degrees. Our method can closely reproduce the 1D and 2D histograms of TGF photons.

While it comes at a high upfront computational cost of collecting the data needed to train it, the resulting cGAN can generate photons at least 1000 times faster than GEANT4 for sources at 12.5km altitude. Overall, our results support the application of machine learning techniques for TGF simulation tasks.

Presenter(s): Pollack, Jianna; Hall, Samanth; McSurdy, Eloise
School: Grinnell College
Session: P1.11
Title: Modeling Elephant Movement with Random Walk Models
Co-Author(s): Jianna Pollack, Owen Gould
Advisor(s): Pratima Hebbar

Abstract: We conducted an in-depth study of modeling elephant movement using random walks, introducing a memory-driven approach called the Adaptive Movement Model (AMM). While we briefly discuss the theoretical foundations of random walks, our primary emphasis is on their application to understanding the behavioral patterns of elephants in Kruger National Park, South Africa. Our analysis identifies two statistically significant behavioral states — 'Encamped' and 'Exploratory' — which are influenced by environmental factors such as precipitation. Our AMM integrates a range of ecological factors influencing elephant behavior, offering a more nuanced representation of their movement dynamics. It incorporates advanced topics in random walks, such as random environments and dependencies based on both location and time. Our research not only enhances the understanding of elephant behavior but also offers valuable insights for conservation strategies. Ultimately, our findings underscore the potential of memory-driven random walk models in capturing the complexities of animal movement in variable environments.

Presenter(s): Restad, Holly
School: Washington University in St. Louis
Session: I.A.4
Title: Aβ(1-40) in a Nanoscale Test Tube; LDAO/10MAG Reverse Micelle Encapsulation of Amyloid Beta
Advisor(s): Yusuke Okuno

Abstract: Amyloid Beta peptide, Aβ(1-40), aggregation is a biomarker of Alzheimer's disease. Insoluble fibrils are well studied; however, toxic oligomers are soluble and transient, making isolating specific oligomer structures a challenge. Confinement of Aβ(1-40) to nanoscale test tubes of controlled size could limit oligomers to a specific species. This project aimed to encapsulate (Aβ1-40) in a reverse micelle system, or "nanoscale test tubes" of 5-15 nm radius, to isolate and characterize the dimeric state. Reverse micelles (RM) are nanoscale droplets of water created in a nonpolar solvent by various surfactant layers. A recently developed system combining LDAO/10MAG surfactants has advantages over similar systems, including retention of the protein's native state and improved NMR performance. Preliminary results show successful RM encapsulation of pure water. Water-to-surfactant concentration ratios were varied to influence RM size. Dynamic light scattering recorded RMs of 20-25 nm diameter at all ratios measured. Future steps involve Aβ(1-40) encapsulation and solution-state NMR. NMR spectroscopy of this LDAO/10MAG RM system can both resolve the dimeric structure and investigate possible drug targets. The introduction of small molecules would allow direct observation of drug-to-dimer interactions.

Presenter(s): Reza Bautista, Oscar

School: Macalester College
Session: P3.07
Title: Exploring ViT and CNN-LSTM Architectures to Aid Indoor Robot Localization and Navigation
Co-Author(s): Susan Fox, Elisa Avalos, Marcus Wallace
Advisor(s): Susan Fox

Abstract: Localization enables robots to determine their position in the world, while navigation involves route planning, speed control, and reaction adjustments based on the environment. Our research aims to improve robot localization by equipping TurtleBots with monocular cameras to predict their location on the second floor of the science building at our college. We explore and compare Convolutional Neural Networks (CNNs) combined with Long Short-Term Memory (LSTM) networks, Vision Transformers (ViTs), and pre-trained CNNs in combination with Transformers for this task. Using a dataset of over 115,000 annotated frames captured from the robot's camera, we evaluate: 1) the reliability of both novel and widely-used architectures, particularly in the context of a relatively small dataset, and 2) strategies for improving datasets for training deep learning models. The CNN-Transformer achieved the highest accuracy for location prediction, with an 81% validation accuracy, while the CNN-LSTM model excelled in direction prediction with 80%. These results provide insights into the effectiveness of different architectures in real-world scenarios, demonstrating the potential for enhancing robot localization and navigation without expensive equipment, making them suitable for low-budget projects. Future work will focus on real-time performance evaluation during robot navigation and the impact of various hyper-parameters on model performance.

Presenter(s): Rosenbaum, Catherine; Beland, Oliver
School: Colorado College
Session: P2.22
Title: Green Solvent Optimization for Solid-Phase Peptide Synthesis of a *Pseudomonas aeruginosa* Prodrug
Co-Author(s): Trenten Chalik, Ty Kruger, Amy Dounay
Advisor(s): Amy Dounay

Abstract: *Pseudomonas aeruginosa* is an opportunistic pathogen that, due to a high degree of antibiotic resistance, commonly affects immunocompromised individuals – particularly those with cystic fibrosis. A prodrug containing 4-fluoro-L-phenylalanine (4-FPhe) designed to target the LecA and LecB enzymes present in *P. aeruginosa* biofilms, minimizes cytotoxicity and maximizes antimicrobial activity. A key component of this prodrug is a pentapeptide containing 4-FPhe. Solid phase peptide synthesis (SPPS) commonly utilizes dichloromethane (DCM) for resin loading, and N,N-dimethylformamide (DMF) for acylation. Both solvents are acutely toxic and hazardous. SPPS optimization focused on identifying green, cost-effective, and accessible solvent alternatives. Resin loading was completed with Acetonitrile/ethyl acetate (EtOAc) (1:1). Previous acylation reactions in EtOAc were inefficient and produced minimal yield. Six binary solvent mixtures with similar polarities to DMF were assessed. Dimethyl sulfoxide (DMSO)/2-methyltetrahydrofuran (2-Me-THF) (3:7) and DMSO/1,3 – dioxolane (DOL) (4:6) significantly improved reaction times and yields.

Presenter(s): Roy, Alexandria
School: Grinnell College
Session: P3.05

Title: Xenon Trapping on Diverse Metal-Supported Silica Nanocages
Co-Author(s): Erik Genet, Shabab Kabir, Jorge Anibal Boscoboinik, Kristen Burson
Advisor(s): Kristen Burson

Abstract: Noble gases are chemically-inert elements, which makes their separation and purification processes expensive and energy-intensive. Alternative techniques of noble gas separation include physically trapping noble gases inside metal-supported nanocages, which has been successfully performed in room-temperature, ultra-high vacuum conditions. In this work, we examine how different metal supports affect xenon trapping in the silica nanocage DodecaPhenyl Polyhedral Oligomeric Silsesquioxane (DP-POSS). DP-POSS was successfully deposited in near-monolayer amounts on Ag(111), Au(111), and Ru(0001) single crystals using a Langmuir-Blodgett trough. Subsequent calcination and reduction of DP-POSS to POSS allows for xenon-trapping capabilities. X-ray photoelectron spectroscopy (XPS) was continuously performed under ultra-high vacuum conditions to investigate the stability of xenon trapped in different stereochemical environments over time. Our results indicate that after initial xenon exposure, gold substrates trapped the highest fraction of xenon per nanocage. All metals lose significant amounts of xenon over time, correlating to xenon located at interstitial sites and xenon trapped in nanocages. Our findings suggest that using different metals allows for customizable noble gas traps, with metal substrates serving as an energy-efficient, less expensive alternative to current industrial-scale noble gas separation methods.

Presenter(s): Ruskin, Daniel
School: Washington University in St. Louis
Session: I.A.2
Title: Mapping Transcription Factor Regulatory Networks in Human Tissues Using Ensemble Learning
Co-Author(s): Wooseok J. Jung, Sandeep Acharya, Shu Liao, Michael R. Brent
Advisor(s): Michael R. Brent

Abstract: Transcription factors are proteins which bind to specific genes and regulate their expression. A major challenge in computational biology is creating networks which connect transcription factors to their target genes in humans. Existing networks tend to lack tissue specificity despite the important role of tissue type in human development and disease processes. Additionally, most networks fail to integrate the full range of datasets needed to infer direct and functional edges between transcription factors and their target genes. In this study, we created transcription factor regulatory networks for an assortment of human tissues. We utilized ensemble machine learning to integrate various data sources, including perturbation, co-expression, motif, and binding data, enabling us to infer direct and functional edges. Our networks outperformed a leading set of human tissue-specific networks on several benchmarks. Ongoing improvements focus on refining data integration to better capture underlying transcription factor regulatory relationships. These preliminary results highlight the potential of ensemble learning for mapping tissue-specific transcriptional regulatory networks in humans. Our networks will contribute to a deeper understanding of the human genome, offering insights into disease formation and gene therapy targets.

Presenter(s): Schneider, Sabrina
School: Washington University in St. Louis
Session: P1.16
Title: Interrogating the Role of the Human Gut Virome in the Development of *Clostridioides*

difficile Infection
Co-Author(s): Kailun Zhang, Vincent Gillespie, Gautam Dantas
Advisor(s): Gautam Dantas

Abstract: *Clostridioides difficile* (*Cd*) infection (CDI) is a gram-positive bacteria that causes inflammation of the colon and clinically significant diarrhea. It is common in the United States, affecting around 500,000 people per year. This disease is difficult to treat because toxigenic *Cd* (T*cd*) can cause diseases from asymptomatic carriage to fatal colitis. Gut bacteriophages are believed to be associated with CDI. This research project aims to understand the role of the gut phageome in T*cd* toxin expression *in vitro*. To accomplish this, viral-like particles (VLPs) were collected from the stool samples of CDI patients and healthy human controls and incubated with *Cd* isolates harboring a reporter plasmid containing the toxin promoter and mCherry fluorescent gene. The fluorescence was used to monitor toxin levels and, therefore, explain how different phageome compositions influence *Cd* infection.

Presenter(s): Scott, Claire
School: Hope College
Session: P2.22
Title: LC/UV-vis and LC/MS/MS to Study the Retinal Carotenoids of Songbirds as a Factor of Habitat and Diet
Co-Author(s): Alison Wegner, Jason Gillmore
Advisor(s): Jason Gillmore

Abstract: The carotenoid-based colors (e.g., bright red, orange, and yellow) of passerine birds are important to honest signaling and sexual selection. While perhaps best known for their role in signaling displays, carotenoids also play an essential role in avian vision, and therefore the sensory perception of the carotenoid displays themselves. In birds, cone photoreceptors contain an oil droplet, a small organelle filled with carotenoids that functions in selectively absorbing certain wavelengths of light and therefore shifting the spectral sensitivity of the cone visual pigments. Birds cannot biosynthesize these carotenoids and must obtain them from their diets. It is our hypothesis that there will therefore be differences in the retinal carotenoids of songbirds based on their habitat, urban or rural. In this very newly launched collaboration, we will apply currently accepted HPLC protocols 1,2 to analyze hydrolyzed retinal carotenoid esters to study this hypothesis. We will simultaneously attempt to develop more robust HPLC/MS/MS methods. With the greater sensitivity and analytical discrepancy of our department's new LC/qTOF instrument (with inline PDA detector for complementary UV-vis analysis), it may be feasible to directly analyze the primary retinal extracts without hydrolysis of the carotenoid fatter acid esters.

Presenter(s): Scott, Liu and Nguyen, Daisy
School: Lawrence University
Session: P1.09
Title: Generic Rigidity of Frames in 3-Space
Co-Author(s): Helin Wang, Mina Mandegar, Liu Scott
Advisor(s): Alexander Heaton

Abstract: We study the combinatorial rigidity of bar-joint frameworks in 3-space. A graph embedded in space is called "rigid" when all other embeddings preserving the edge-lengths are rigid motions of Euclidean space, meaning translations, rotations, or reflections. A graph is called "flexible" otherwise, since a one-parameter family of embeddings which do not arise from rigid

motions may be visualized as a physically realizable structure deforming and losing its shape. In particular, we study the X-replacement and double-V replacement conjectures. These graph operations are conjectured to preserve rigidity. We verified the non-existence of counterexamples on graphs with less than 15 vertices computationally. Finally, we also provided explicit proofs of the "reverse" 2-extension theorem which makes the X and double-V replacements so important.

Presenter(s): Seo, Eric
School: Beloit College
Session: I.C.3
Title: Optimized White Sox Lineup Construction with Machine Learning Ensemble Model and Monte-Carlo Game Simulation
Co-Author(s): Aniyah McWilliams, Neal Lim
Advisor(s): Katherine Harris

Abstract: Traditional baseball lineup strategies often rely on intuition and basic statistics. However, with advancements in data analytics and machine learning, there is potential to enhance these strategies through various mathematical techniques.
Using a comprehensive dataset of play-by-play event files, our approach leverages a machine learning ensemble model to predict at-bat outcomes and simulate game results. The model integrates various player performance metrics, situational factors, and game contexts to analyze lineup performance. By running Monte-Carlo simulations, the model identifies lineups that maximize the team's predicted run count, providing a data-driven approach to lineup optimization.

Presenter(s): Shirley, Gabrielle and Stewart, Isaac
School: Hope College
Session: P2.16
Title: Biodegradable Metallopolymers: Kinetic Studies on the Polymerization of Cyclic Carbonate Monomers with Pendant Metallocenes
Co-Author(s): Christopher Turlington
Advisor(s): Christopher Turlington

Abstract: The library of cyclic trimethylene carbonate monomers with pendant organic functional groups continues to grow. Polymerization yields biodegradable polycarbonates with tailored properties. However, transition metal functional groups pendant to the carbonate monomer are essentially unexplored. Can polycarbonates with pendant metallocenes by synthesized using organocatalytic ring-opening polymerization? The answer is yes, when an appropriate linker is chosen to connect the cyclic carbonate to the metallocene. Ferrocene-carbonate and ruthenocene-carbonate monomers are synthesized. Controlled homopolymerizations are possible at room-temperature, which is unusual for the metallopolymer field. A diblock copolymer is synthesized with the two metal-carbonate monomers, and diblock copolymers are also synthesized with the ruthenocene-carbonate monomer and a strictly organic carbonate monomer. The pendant metallocenes could add useful new properties to biodegradable polycarbonate backbones, such as redox activity and light absorption/emission.

Presenter(s): Short, Whitney
School: Washington University in St. Louis
Session: I.B.3
Title: Quantum Algorithms for Modeling Open Quantum Systems at Temperature with the

Bloch-Redfield Equation
Co-Author(s): Koray Aydogan, Mikayla Fahrenbruch, Timothy J. Krogmeier, Maryam Abbasi, Anthony W. Schlimgen, Kade Head-Marsden
Advisor(s): Kade Head-Marsden

Abstract: Behavior in many quantum systems relevant to present chemistry and materials science is driven by interaction with an external environment. Quantum algorithms are a useful tool to study the evolution of these open quantum systems, but presently, the majority of these algorithms can only model behavior at low temperature. The Bloch-Redfield equation, conversely, offers the ability to examine thermodynamically produced dynamics in open systems, allowing us to access observables pertaining to temperature. Here, we investigate how the Bloch-Redfield equation can be implemented to model open quantum systems on current quantum computers. Current hardware can only implement unitary gates, so we map the non-unitary Bloch-Redfield operations into unitary ones, providing a mode to model non-unitary behavior at temperature on a quantum computer. As this process can be costly, we optimize the circuits and operator decompositions by taking advantage of often present characteristics like sparsity and symmetry.

Presenter(s): Singh, Navraj
School: Lawrence University
Session: P3.17
Title: Novel Gold Catalyzed Synthesis of 1H-Isochromenes
Co-Author(s): Miles McCue, Juliana Mouat, Zach Grimm, Mike Gesinski
Advisor(s): Mike Gesinski

Abstract: 1H-isochromene belong to a larger family of molecules called benzopyrans which are prolifically used in the pharmaceutical industry. Production of these molecules is challenging due to the preference of most nucleophiles to form the benzofuran product. Presented here is a novel synthesis producing 1H-isochromene through a two-step, mild synthesis. The scheme entails a standard Sonogashira cross coupling reaction followed by a regioselective, gold catalyzed cyclization to produce the benzopyran product. The cyclization occurs through a 6-endo-dig pathway because the benzylic gold-alkene intermediate formed post nucleophilic attack is kinetically favored. In addition to producing a valuable product, this mild, regioselective reaction has far reaching implication to produce other valuable products.

Presenter(s): Solomon, Sarah
School: Macalester College
Session: P2.18
Title: 1,2,3 Triazole Synthesis and Reaction
Co-Author(s): Hazel Waters, Kaitlyn Pistorius, Ronald Brisbois
Advisor(s): Ronald Brisbois

Abstract: The 1,2,3-triazole scaffold is an important pharmacophore and a versatile, increasingly leveraged, substructure in biochemical, materials, polymer, and metal-coordinating applications. Continuing advances in 1,2,3-triazole construction, by either non-catalyzed or metal-catalyzed azide/alkyne cycloaddition, foster further creative use. Previously, the Brisbois Lab has optimized a protocol for reacting bis(trimethylsilyl)butadiyne with azides to form 5-trimethylsilylethynyl-4-trimethylsilyl-1,2,3-triazoles in good to excellent yield. Scott Pederson (‘19) furthered this work by using an indole triazole to form a new molecule containing a

7-membered ring featuring an exomethylene. We explored the potential of this exomethylene by conducting hydrogenation and ozonolysis reactions to varying degrees of success. Additionally we attempted “Scott’s reaction” on an additionally substituted benzyl bromide, which did not form the analogous 7-membered ring structure that was found with the indole triazole. We have begun to explore the desilylation of our triazole products for the purpose of synthesizing N-Unsubstituted Bis Triazoles, with mixed results.

Presenter(s): Steineke, Teagan and Wheeler, Justin
School: Carthage College
Session: P1.02
Title: Towards the Response of Discontinuous Linear Systems to Stationary Random Excitation for Ullage Detection
Co-Author(s): Justin Wheeler, Jordan Wheeler, Sikiel Graves, Owen Bonnett
Advisor(s): Kevin Crosby

Abstract: A stationary material surface divided into two regions with a mass discontinuity under random excitation will exhibit a change in the mean square response of displacement and velocity at the discontinuity. As surface waves propagate across the interface between regions, they encounter the impedance mismatch arising from the added mass at the boundary, and part of the wave energy is reflected, while part of the wave is transmitted across the interface. This mechanism can be exploited to measure the location of the liquid-vapor interface in a liquid propellant tank by measuring the mean square response of the material surface along the tank wall. The generalized case for simple stationary geometries with a mass discontinuity under random excitation at a localized source has been solved previously. However, liquid propellant tanks are often conformal geometries, and the theory for these complex systems is still at an early stage. We present the efforts towards a comprehensive analytical theory of the physical mechanism that underlies the Microgravity Ullage Detection project.

Presenter(s): Stewart, Isaac and Shirley, Gabrielle
School: Hope College
Session: P2.16
Title: Biodegradable Metallopolymers: Kinetic Studies on the Polymerization of Cyclic Carbonate Monomers with Pendant Metallocenes
Advisor(s): Christopher Turlington

Abstract: The library of cyclic trimethylene carbonate monomers with pendant organic functional groups continues to grow. Polymerization yields biodegradable polycarbonates with tailored properties. However, transition metal functional groups pendant to the carbonate monomer are essentially unexplored. Can polycarbonates with pendant metallocenes by synthesized using organocatalytic ring-opening polymerization? The answer is yes, when an appropriate linker is chosen to connect the cyclic carbonate to the metallocene. Ferrocene-carbonate and ruthenocene-carbonate monomers are synthesized. Controlled homopolymerizations are possible at room-temperature, which is unusual for the metallopolymer field. A diblock copolymer is synthesized with the two metal-carbonate monomers, and diblock copolymers are also synthesized with the ruthenocene-carbonate monomer and a strictly organic carbonate monomer. The pendant metallocenes could add useful new properties to biodegradable polycarbonate backbones, such as redox activity and light absorption/emission.

Presenter(s): Suelflow, Kyle

School: Macalester College
Session: P3.09
Title: Age Heaping in Probability Surveys in Sub-Saharan Africa: Frequency and Consequences for Mortality Estimation
Co-Author(s): Taylor Okonek
Advisor(s): Taylor Okonek

Abstract: Estimates of under-5 mortality rates (U5MR) are an important indicator of the health of a country. In low- and middle-income countries (LMICs), estimates of U5MR primarily come from probability surveys as opposed to vital registration systems or censuses. The most prevalent of such surveys are the Demographic and Health Surveys (DHS), which are known to have certain quality concerns endemic to probability surveys. One of these quality concerns is age heaping, where a disproportionate number of child deaths are reported at rounded ages, such as 12 months. The exact frequency of age-heaping in DHS surveys is not well-studied, and its impacts on downstream statistical analyses---in particular, the estimation of summary measures of mortality---has not been rigorously explored. We investigate the prevalence of age heaping in DHS surveys from sub-Saharan Africa by conducting simulations with various "severities" of age heaping, and assessing the impact of age heaping on commonly used statistical methods for estimating child mortality summary measures in settings akin to those found in LMICs.

Presenter(s): Thibodeaux, Douglas
School: Washington University in St. Louis
Session: P1.20
Title: Nested Sampling for Noble Gas Adsorption on Graphene
Co-Author(s): Douglas Thibodeaux, Mingrui Yang, and Robert B. Wexler
Advisor(s): Robert Wexler

Abstract: Using nested sampling, we examined the thermodynamic properties of low-coverage argon monolayers adsorbed onto a graphite slab. Calculated values of heat capacity vs. temperature were compared to the results of previous experimental and computational studies to determine the effectiveness of nested sampling in modeling real chemical systems. The calculated heat capacity curves show two peaks. One of these peaks corresponds to a transition between a liquid and a condensed droplet phase, and the other corresponds to a transition between the condensed droplet and an ordered solid phase. These peaks are also seen in previous studies, indicating that nested sampling can accurately capture these types of transitions. An additional peak is missing from the nested sampling heat capacity curves present in experimental and other computation studies, which corresponds to an orientational transition of the argon layer. Molecular dynamics simulations of this system indicate the presence of a rotated ground state for large sets of particles; however, currently, available packages for performing nested sampling simulations are not able to carry out simulations of adequate sizes, suggesting that nested sampling may not be the most effective tool for exploring these types of transitions.

Presenter(s): Thompson, Kiely
School: Knox College
Session: P3.14
Title: Synthesis of Phosphonate Estolides from Castor Oil
Advisor(s): Diana M. Cermak

Abstract: Bio-based oils offer a sustainable alternative to more widely used petroleum-based oils

and fuels, but have often lacked performance in cold temperatures. Estolides are a recent class of bio-based oils that are synthesized from oils derived from plants and have shown very good low temperature properties. An estolide is an ester functional group that can be produced from fatty acids and fatty acid esters. A variety of estolides have been created using Castor oil, from the plant Ricinus communis, and a saturated capping material, which are saturated fatty acids. Castor oil mainly contains the fatty acid ricinoleic acid, and estolides have been synthesized from the whole castor triglyceride and from fatty acid derivatives, yet no estolide has yet been synthesized which contain a phosphonate group. The Cermak lab has synthesized many phosphonate-containing derivatives of Castor oil, so the addition of a phosphonate to an estolide is a natural extension of our previous work. The purpose of this research aims at synthesizing a phosphonate-containing estolide from ricinoleic acid of Castor oil, using lauric acid as the capping material and a hydroxy phosphonate. The progress towards the synthesis of the phosphonate estolide will be presented.

Presenter(s): Torgelson, Claire
School: Grinnell College
Session: I.B.4
Title: Variable Temperature Diffusion in Mixed Anion Electrolytes for Lithium and Lithium-Ion Batteries
Co-Author(s): Ryan Boev and Leslie J. Lyons
Advisor(s): Leslie J. Lyons

Abstract: Seeking better low temperature electrolyte performance, we report on multi-nuclear pulsed field gradient (PFG) NMR experiments over the temperature range of -20 ^{o}C to 40 ^{o}C. We have used two different anions, PF6- and FSI- in an effort to improve lithium ion diffusion over this temperature range. The base electrolyte was 1 M lithium salt in a solvent blend of equal proportions of ethylene carbonate, diethyl carbonate, and ethyl methyl carbonate with the additive vinylene carbonate. Multinuclear 1H, 7Li, and 19F pulsed field gradient NMR experiments over this temperature range measure the slowest diffusion for the lithium cation and increasing diffusion coefficients, respectively, for the anion, the ethylene carbonate protons, the diethyl carbonate protons and the fastest diffusion coefficient for the ethyl methyl carbonate solvent component. In mixed anion electrolytes the diffusion coefficient for the FSI anion is consistently larger than the PF6 anion with the largest increase in the diffusion coefficient of the anion at -20 ^{o}C. We will also report on the salt dissociation values and lithium transport numbers for these electrolytes. The increased diffusion characteristics of LiFSI enhance electrolyte performance, and blends of LiFSI and LiPF6 may optimize lithium-ion battery results, especially at low temperatures.

Presenter(s): Tsang, Chloe Isabella
School: University of Chicago
Session: II.F.1
Title: Design and Implementation of an Inductively Coupled Plasma Source
Co-Author(s): Ivy Chen
Advisor(s): Dr. Austin J. Minnich

Abstract: Inductively Coupled Plasmas (ICPs) are highly ionized gases generated by electromagnetic fields, commonly used in various nanofabrication processes due to their high ion density and uniformity. ICPs are key in applications such as etching and deposition, where precise control over material removal or addition is needed. In this project, ICPs are utilized for

Atomic Layer Etching (ALE), a process that allows for the atomic-scale precision etching of materials. We have designed and constructed a custom ICP source, aimed at advancing ALE techniques. Starting with a conceptual design, we identified and sourced all necessary components, ensuring compatibility and functionality. The design process included detailed research on plasma generation, power supply requirements, and the configuration of the ICP system. After procuring the components, we assembled the system while addressing challenges related to component integration and operational stability. The resulting ICP source aims to demonstrate effective plasma generation, providing a key component for precise and controlled ALE processes.

Presenter(s): Valentini, Andrew
School: Carthage College
Session: I.B.2
Title: Non-Completely Positive Dynamics as a Probe of Entanglement in Quantum Circuits
Advisor(s): Sarah Shandera

Abstract: Motivated by the possible information to be gained from studying the evolution of ensembles of interacting quantum systems in a cosmological context, we develop a simulation of a quantum circuit. We treat the full circuit as an ensemble of open systems and track the state of these subsystems as correlations between them develop. We use violations of complete positivity on the mappings that evolve subsystems as a diagnosis for entanglement in the circuit and study the domain of positivity for these mappings to determine between which subsystems the entanglement exists at a given time. We additionally define thermodynamic properties such as relative entropy and the change in extractable work of the subsystems and investigate their relationship to the non-positive maps. This is carried out for circuits of varying interaction to further reveal the ability of mappings to probe the evolution of entanglement and thermodynamic properties.

Presenter(s): Vega Juarez, Itzel
School: Lawrence University
Session: P3.15
Title: Synthesis and Characterization of NDI-TTM2•
Co-Author(s): Graham Sazama
Advisor(s): Graham Sazama

Abstract: In this project, we are trying to find molecules with doublet ground states, that is, radicals, that can luminesce and are stable at the same time. I outline my work in pursuit of the molecule NDI-TTM2, a potential luminescent radical fusing the radical framework tris(2,4,6 trichlorophenyl)methyl (TTM) and the chromophore naphthalene diimide (NDI). To synthesize this molecule, we started by making the radical TTM. In order to have a double substitution of our radical into naphthalene tetracarboxylic dianhydride (NDA), our NDI synthon, we substitute a *para*- chlorine of the TTM radical with an amine group through the use of antimony pentachloride (SbCl5). We were able synthesize NH2-TTM; and are now working on purification. This is a critical step toward our goal of synthesizing NDI-TTM2 and testing for its efficiency of luminescence.

Presenter(s): Vizoso-Marino, Miranda and Monroe, Frances
School: Gustavus Adolphus College
Session: P2.08

Title: Environmental Controls on Stromatolite Morphology in the Ordovician Prairie Du Chien Group
Co-Author(s): Frances Monroe, Julie Bartley
Advisor(s): Julie Bartley

Abstract: Stromatolites are organo-sedimentary structures that grow on carbonate platforms. Stromatolite form, at both macro and meso scale is sensitive to changes in the environment. However, the specific ways that environmental factors shape stromatolite morphology remain largely unknown. The stromatolites of the Ordovician Prairie du Chien Group are well-exposed in Minnesota and Wisconsin, and their patterns and changes in both mesostructure and macrostructure may record environmental change in ancient oceans. Multiple field sites in both Minnesota and Wisconsin were visited to investigate stromatolite morphological variability. To investigate the causes of mesostructure change, individual laminae of stromatolites from the Prairie du Chien Group were traced, revealing that the introduction of sand to a stromatolite disturbs stromatolite growth, causing lower inheritance. At the macroscale level, we observed that stromatolites in the upper half of the Prairie du Chien Group are characterized by a transition from small domal layered stromatolites to large, flat-laminated forms. This pattern probably records a shoaling upwards sequence. However, the lower half of the Prairie du Chien Group does not exhibit that same morphological pattern. This difference in macroscale pattern raises a question: what environmental differences separate the lower and upper parts of the Prairie du Chien Group?

Presenter(s): Wang, Helin and Mandegar, Mina
School: Lawrence University
Session: P1.08
Title: Generic Rigidity in 3-Space
Co-Author(s): Daisy Nguyen, Mina Mandegar, Liu Scott, Alexander Michael Heaton
Advisor(s): Alexander Michael Heaton

Abstract: We study the combinatorial rigidity of bar-joint frameworks in 3-space. A graph embedded in space is called "rigid" when all other embeddings preserving the edge-lengths are rigid motions of Euclidean space, meaning translations, rotations, or reflections. A graph is called "flexible" otherwise, since a one-parameter family of embeddings which do not arise from rigid motions may be visualized as a physically realizable structure deforming and losing its shape. In particular, we study the X-replacement and double-V replacement conjectures. These graph operations are conjectured to preserve rigidity. We verified the non-existence of counterexamples on graphs with less than 15 vertices computationally. Finally, we also provided explicit proofs of the "reverse" 2-extension theorem which makes the X and double-V replacements so important.

Presenter(s): Wang, Sean and Avula, Rohan
School: Washington University in St. Louis
Session: P1.12
Title: Improving the Dynamic Sensitivity of Plasmonically Enhanced Immunoassays
Co-Author(s): Yixuan Wang, Rohit Gupta, Ananya Benegal, Michael D. Vahey, Srikanth Singamaneni
Advisor(s): Srikanth Singamaneni

Abstract: For improving the ultrasensitive and quantitative detection of low-abundance biomarkers on standard immunoassays, many groups have attempted to improve the sensitivity

of the fluorophore or nanoparticle used. In addition to better reporter elements, a rarely discussed, yet crucial limitation to sensitivity is analyte bulkiness and binding orientation. We explore two inexpensive and effective improvements: high-avidity synthetic antibodies and cyclic draining and replenishing technology (CDR) to improve the dynamic sensitivity of plasmonic-fluor based lateral flow assays (p-LFA) and immunosorbent assays (p-FLISA). Our high-avidity synthetic antibody improves the sensitivity of p-LFAs by optimizing analyte binding orientation through multivalent binding afforded by conjugating LCB1 affibodies (antibody mimetic miniproteins) to bovine serum albumin (BSA). Due to the size of Plasmonic Fluor, steric hindrance effects limit antigen binding and sensitivity. CDR uses periodic rotation of the assay to promote binding efficiency of the PF reporter element for both the sandwich assay and competitive ELISA. Overall, we report significant improvements in sensitivity in immunoassays through the novel application of various techniques.

Presenter(s): Weeda, Hope
School: Hope College
Session: P1.04
Title: Effect of Energy-Dependent Proton Irradiation on Thin-Film YBa2Cu3O7−δ Superconductor
Co-Author(s): Joey Fogt, Nolan Miles, Trevor Harrison, Kyuil Cho
Advisor(s): Kyuil Cho

Abstract: In prior research we investigated the effect of 0.6 MeV proton irradiation on the superconducting and normal-state properties of thin-film YBa2Cu3O7−δ superconductors and found that the relationship between the critical temperature and dimensionless scattering rate obtained during proton irradiation approximated the generalized d-wave Abrikosov–Gor'kov theory better than the previous results obtained from electron irradiations. This was unexpected, as electron irradiation is generally thought to be more effective than heavier ion irradiation at suppressing superconductivity. We reasoned that 0.6 MeV protons can produce point-like defects with an implantation depth much longer than the sample thickness, and that proton irradiation is more uniform in causing defects across all element sites. To test this hypothesis, a thin-film YBa2Cu3O7−δ superconductor was irradiated with 1.7 MeV proton irradiation, and results will be shared at the conference.

Presenter(s): Weissling, Emma
School: Hope College
Session: P2.03
Title: Beta-Decay Feeding Intensity Distribution of 93Rb
Co-Author(s): Paul DeYoung, Artemis Spyrou, Belen Monteagudo, William von Seeger
Advisor(s): Paul DeYoung

Abstract: Many astrophysical processes require as input beta-decay properties of exotic nuclei. In many cases, such as in the r-process, the relevant nuclei are not yet accessible by current facilities, and astrophysical models use theoretical calculations to describe the relevant beta decays. It is, therefore, critical to have complete measurements, where possible, that can be used to constrain theoretical calculations. In the present work we focus on the study of the beta-decay of the neutron-rich isotope 93Rb. A 93Rb beam was produced at the National Superconducting Cyclotron Laboratory (NSCL). 93Rb nuclei were implanted in a mylar tape. The electrons from the β decay were measured in a plastic scintillating barrel-shaped β detector, while the γ rays were detected in the Summing NaI(Tl) (SuN) detector. The β-decay strength function was measured with the technique Total Absorption Spectroscopy. The results are compared to

beta-decay models commonly used in astrophysical calculations.
Presenter(s): Wheeler, Jordan; Bonnett, Owen; Graves, Sikiel
School: Carthage College
Session: P1.01
Title: Validating an Ullage Detection Technique for Liquid Propellant Tanks
Co-Author(s): Justin Wheeler, Sikiel Graves, Owen Bonnett, Teagan Steineke
Advisor(s): Kevin Crosby

Abstract: The Microgravity Ullage Detection (MUD) experiment is an element of a larger effort to address ullage venting during in-space refueling operations. Carthage College, in collaboration with the Johnson Space Center Power and Propulsion division, is developing technologies to locate the ullage bubble in a propellant tank and to facilitate the venting of ullage gas during refueling. The MUD payload has two primary technical objectives: (1) demonstrate that, under gravity, a liquid-vapor interface can be detected non-invasively using external acoustic patch sensors mounted on the tank, and (2) demonstrate that, under microgravity, changes in the thickness of the adhered liquid layer can be measured non-invasively during a tank drain using external acoustic patch sensors mounted on the tank. Ullage detection is accomplished by exploiting the fact that the sensor output is sensitive to the local stiffness and damping of the tank wall. By calculating the Root Mean Square of the sensor at a given location, liquid presence and interface velocity at the location of the sensor can be inferred, thus identifying the location and geometry of the ullage. Under gravity, the location of fluid interface has been determined with resolution of < 1% of the full-tank volume for settled liquids.

Presenter(s): Wheeler, Justin and Steineke, Teagan
School: Carthage College
Session: P1.02
Title: Towards the Response of Discontinuous Linear Systems to Stationary Random Excitation for Ullage Detection
Co-Author(s): Jordan Wheeler, Teagan Steineke, Sikiel Graves, Owen Bonnett
Advisor(s): Kevin Crosby

Abstract: A stationary material surface divided into two regions with a mass discontinuity under random excitation will exhibit a change in the mean square response of displacement and velocity at the discontinuity. As surface waves propagate across the interface between regions, they encounter the impedance mismatch arising from the added mass at the boundary, and part of the wave energy is reflected, while part of the wave is transmitted across the interface. This mechanism can be exploited to measure the location of the liquid-vapor interface in a liquid propellant tank by measuring the mean square response of the material surface along the tank wall. The generalized case for simple stationary geometries with a mass discontinuity under random excitation at a localized source has been solved previously. However, liquid propellant tanks are often conformal geometries, and the theory for these complex systems is still at an early stage. We present the efforts towards a comprehensive analytical theory of the physical mechanism that underlies the Microgravity Ullage Detection project.

Presenter(s): Whittaker, Kaisa
School: Gustavus Adolphus College
Session: P2.09
Title: Human Conflict and Soil Erosion, Environmental and Land Use Change Within the Early Modern Period

Co-Author(s): Kendall Wiggins, Erik L Gulbranson
Advisor(s): Erik L Gulbranson

Abstract: Soil erosion occurs globally, reshaping landforms and reducing soil quality. Knowledge of soil erosion from human activity is vast. Significant gaps remain, however, such as the effects of conflict on soil erosion. This study will develop an understanding of how conflict affects soil erosion by establishing the effects of conflict during Europe's early Modern period. Field data and samples from sedimentary archives of floodplain strata reveal pedogenically modified alluvial deposits interspersed with colluvium. A landscape equilibrium index assesses landscape age against soil residence time. Analysis indicates modern soils are closer to equilibrium than buried soils, indicating the buried soils were more susceptible to erosion. A new model for Soil Erosion, Discharge, and Slope (SEDS) reconstructs these parameters, and indicates that slope has decreased from the past, with the greatest change in highest order streams. These streams have reconstructed power beyond the stream erosion threshold, indicating bank erosion had a significant role. Streams with lower discharge display more erosion sensitivity to rainfall intensity, indicating spatial variability in the processes controlling soil erosion. Work on stratigraphic age and colluvium provenance establishes the temporal connection of these results to conflict, and the connection between bank erosion and slope movements of soil material, respectively.

Presenter(s): Wiggins, Kendall
School: Gustavus Adolphus College
Session: P2.09
Title: Human Conflict and Soil Erosion, Environmental and Land Use Change Within the Early Modern Period
Co-Author(s): Kaisa Whittaker, Erik L Gulbranson
Advisor(s): Erik L Gulbranson

Abstract: Soil erosion occurs globally, reshaping landforms and reducing soil quality. Knowledge of soil erosion from human activity is vast. Significant gaps remain, however, such as the effects of conflict on soil erosion. This study will develop an understanding of how conflict affects soil erosion by establishing the effects of conflict during Europe's early Modern period. Field data and samples from sedimentary archives of floodplain strata reveal pedogenically modified alluvial deposits interspersed with colluvium. A landscape equilibrium index assesses landscape age against soil residence time. Analysis indicates modern soils are closer to equilibrium than buried soils, indicating the buried soils were more susceptible to erosion. A new model for Soil Erosion, Discharge, and Slope (SEDS) reconstructs these parameters, and indicates that slope has decreased from the past, with the greatest change in highest order streams. These streams have reconstructed power beyond the stream erosion threshold, indicating bank erosion had a significant role. Streams with lower discharge display more erosion sensitivity to rainfall intensity, indicating spatial variability in the processes controlling soil erosion. Work on stratigraphic age and colluvium provenance establishes the temporal connection of these results to conflict, and the connection between bank erosion and slope movements of soil material, respectively.

Presenter(s): Xu, Emily
School: University of Chicago
Session: P3.03
Title: Differentiating Healthy Aging, Early, and Intermediate Age-Related Macular Degeneration via Retinal Thickness in Optical Coherence Tomography - ALSTAR2 Baseline

Co-Author(s): Emily Xu, Kenzie Megid, Sophia Xu, Sohaib Fasih-Ahmad, Ziyuan Wang, Zubin Mishra, Mark Clark, Thomas Swain, Christine Curcio, Cynthia Owsley, SriniVas Sadda, Zhihong Jewel Hu*
Advisor(s): Zhihong Jewel Hu

Abstract: Retinal layer thickness features may be affected by age-related macular degeneration (AMD) processes. The purpose of this project is to investigate associated retinal layer thicknesses in optical coherence tomography for differentiation of healthy aging, early, and intermediate AMD. The study included 371 total eyes (133 early AMD, 17 intermediate AMD, and 221 normal from subjects ≥ 60 years) [1]. An automatic segmentation algorithm was applied [2-4] to obtain internal limiting membrane boundary, inner nuclear-outer plexiform junction, and inner and outer choroidal boundaries [5-6]. Each B-scan was manually inspected and refined if needed. The analysis was with 3-6mm, 1-3mm ring, and within 1mm ETDRS rings in inner retinal, outer retinal, and choroid. With an ANOVA test, there was a significant ($p<0.05$) difference among AMD stages within 1mm and 1-3mm ring of inner retinal. With a T-test between normal and early AMD, there was a significant difference in all inner retinal and 3-6mm ring of choroid. Likewise, when comparing normal to intermediate AMD and intermediate to early AMD, there was a significant difference in outer retinal within 1mm ring. Overall, most significant differences were found in all inner retinal, within 1mm ring of outer retinal, and 3-6mm ring of choroid.

Presenter(s): Xue, Yuji
School: Macalester College
Session: II.E.2
Title: Investigating Odorant Receptor Enantiomer Discrimination Mechanism
Co-Author(s): Ichie Ojiro
Advisor(s): Hiro Matsunami

Abstract: The perception of smell starts from binding between volatile odor molecules and olfactory receptors expressed in the olfactory epithelium. These receptors are activated and initiate signals. Studies have shown that most vertebrate species, such as humans, are able to discriminate a variety of odrants based on combinatorial activation of olfactory receptors. Using a coding mechanism, humans can distinguish a variety of smells, even enantiomers. Despite their similarities, previous studies have shown that humans are able to distinguish the smell between enantiomers. However, the detailed molecular mechanism of odor discrimination is still unclear. To answer this question, our research focused on investigating the enantiomer discrimination of olfactory receptors and exploring the underlying stereoselectivity mechanisms using both high through output in-vitro assay and molecular dynamic simulation.

Presenter(s): Yan, Yiwei and López González, Mariela
School: Grinnell College
Session: P3.04
Title: Bulk Refractive Index Sensitivity of LSPR Sensors on Substrate
Co-Author(s): Mariela Lopez Gonzalez; Keisuke Hasegawa
Advisor(s): Keisuke Hasegawa

Abstract: Localized surface plasmon resonance (LSPR) biosensors are a popular label-free detection method for detecting biological molecules. These sensors rely on the optical properties of metal nanoparticles (NPs) and the collective oscillation of their free electrons upon incident waves. LSPR sensors include in-suspension and on-substrate, where the latter has not been

extensively studied. Building on the understanding of substrate-nanoparticle interactions is important for the design of on-substrate sensors. We theoretically investigate the bulk refractive index (RI) sensitivity of immobilized gold NPs of various geometries (square, disk, hexagon, cuboid, cylinder, triangle, and rod). Using MNPBEM, a MATLAB toolbox, we verify that the effect of the substrate on the RI sensitivity is dependent on the NP shape. The smallest decrease in the bulk RI sensitivity is seen for nanorod and nanocylinder, whereas plate-like shapes show a significant decrease in the sensitivity once immobilized. We combine effective medium and quasistatic theory to derive an analytical expression for predicting the sensitivity. The expression presents the best accuracy for rod and cylinder shapes. The low-impact substrate effect and high theoretical accuracy make these NP geometries suitable for sensor design.

Presenter(s): Zhu, Guanchen
School: University of Chicago
Session: P3.19
Title: Asymmetric Total Synthesis of Bipolarolide A-B
Co-Author(s):
Advisor(s): Scott A. Snyder

Abstract: Bipolarolide A and B, two sesterterpenes isolated from Bipolaris sp. TJ403-B, exhibit a novel caged 5/6/6/6/5 pentacyclic skeleton with two contiguous quaternary centers. Biologically, in vitro assays revealed that Bipolarolide A demonstrates remarkable hypolipidemic activity, inhibiting HMG-CoA reductase with an IC50 value of 2.46 ± 0.07 μM. Driven by the complexities and biological activities of these molecules, we report here our synthetic efforts toward the common core of Bipolarolide A and B in 15 linear steps. Key steps in our asymmetric total synthesis include a chiral auxiliary-assisted asymmetric Birch reduction, a hetero Diels-Alder cycloaddition, a gold(I)-catalyzed Ene reaction, followed by an Aldol condensation, and concluding with a SmI2-mediated aldehyde-alkene coupling to yield the core structure of the target molecules. Notably, our synthesis features a mild gold(I)-catalyzed Ene reaction between an alkene and an alkyne, generating a quaternary stereocenter. This reaction is particularly advantageous for acid- and base-sensitive compounds and holds potential for application in the synthesis of other natural products with quaternary centers, such as waihoesene and Bipolarolide C-D. By following the synthetic route previously reported by the Yanxing Jia group, we anticipate completing the synthesis in an additional 7 steps.

Students Presenting at
MCMS Undergraduate Research Symposium,
Washington University in St. Louis
Physical Sciences, Math and Computer Science
November 15-16, 2024

Beloit College: Vu-Anh Le, Eric Seo

Carthage College: Juliana Alvarez, Owen Bonnett, Iman Deanparvar, Frannie Drake, Skylar Farr, Dawson Gaynor, Sikiel Graves, Lucas Peterson, Teagan Steineke, Andrew Valentini, Jordan Wheeler, Justin Wheeler

Colorado College: Ollie Beland, Trenten Chalik, Sabra Catalano, Patrick Loos, Cate Rosenbaum

Grinnell College: Ian Clawson, Mariela López González, Sam Hall, Shabab Kabir, Hannah Kim, Eloise McSurdy, Clare O'Brien, Jianna Pollack, Andrea Roy, Claire Torgelson, Vivien Yan

Gustavus Adolphus College: Samantha Anderson, Erin Coleman, Arya Menk, Miranda Vizoso-Marino, Fran Monroe, Ronard Pabi, Kaisa Whittaker, Kendall Wiggins

Hope College: Bishop Carl, Ethan De Koker, John Levering, Teague Merrill, Claire Scott, Gabrielle Shirley, Isaac Stewart, Hope Weeda, Emma Weissling, Henry Westphal

Knox College: Ridham Dholaria, Franny Hilliard, Naysha Jain, Jack Lubbs, Precious Odejimi, Santosh Pant, Kiely Thompson

Lawrence University: Mina Mandegar, Daisy Nguyen, Liu Scott, Navraj Singh, Itzel Vega Juarez, Helin Wang

Macalester College: James Bradley, Dana Hicks, Lindsay Monkam, Sydney Ohr, Oscar Reza Bautista, Sarah Solomon, Kyle Suelflow, Yuji Xue

St Olaf College: Mackenzie Amann, Matthew Blake, Liam Gallagher, Pauline Iwerks, Eva McKinney, Matthew Oberlander

University of Chicago: Maryam Adebisi, Meera Dasgupta, Pierce Hoenigman, Hannah Parish, Chloe Isabella Tsang, Emily Xu, Guanchen Zhu

Washington University in St, Louis: Rohan Avula, Caroline Cramer, Charlie Fioriglio, Amanda Gary, Tatum Goforth, Ronan Hanley, Phoenix Jarosz, Archer Li, Dongting Li, Thomas Li, Sydney Mayer, Cassidy Metzger, Jasmine Najari, Holly Restad, Daniel Ruskin, Sabrina Schneider, Whitney Short, Douglas Thibodeaux, Sean Wang

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MCMS Undergraduate Research Symposium,
Washington University in St. Louis
Physical Sciences, Math and Computer Science
November 15-16, 2024

John Bleeke, Washington University in St. Louis, Chemistry Department

Murphy Brausel, Colorado College, Chemistry Department

David Brownholland. Associate Professor, Carthage College, Department of Chemistry

Kristen Burson, Associate Professor, Grinnell College, Department of Physics

Darsa Donelan. Senior Continuing Faculty. Gustavus Adolphus College, Department of Physics

Paul Fischer, Professor, Department of Chemistry, Macalester College

Francesca Gandini, Assistant Professor. St. Olaf College, Department of Mathematics

Michael Gerten. Assistant Professor, Department of Computer Science, Knox College

Katherine Harris. Assistant Professor, Department of Mathematics, Beloit College

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Lee Sharpe. Professor, Department of Chemistry, Grinnell College

Scott Snyder, Professor, University of Chicago, Chemistry Department

Tim Wencewicz, Professor, Washington University in St. Louis, Director of Graduate Studies

Graduate Student Panel

Anna Hartig, Wooster College graduate
April Lopez, Beloit College graduate
Diego Lopez Gutierrez, Macalester College graduate
Evan Schultheis, Grinnell College graduate
Wesley Wagner**,** Wooster College graduate