The 2021 University of Chicago Undergraduate Research Symposium: Online Proceedings

Virtual Poster Session 1:

Physical Sciences Collegiate Division
Algorithmic Design of Dynamic Control Sequences for Protecting Quantum Bit Coherence
Ahmed Malik, 2nd-Year, Physics
Mentor(s): Prof. Tian Zhong, Pritzker School of Molecular Engineering

Quantum computers use the principle of superposition to store combinations of 0s and 1s called qubits. Through entanglement, qubits can be inextricably linked so that changing the state of one qubit instantaneously affects its entangled partner. These properties allow quantum computers to step in where traditional computers struggle, namely computationally intense tasks in AI, molecular design, financial technology, cryptography, and more. However, qubits suffer from decoherence: the decay of a superposition due to environmental interference. The feasibility of quantum computing predicates on a long-lived decoherence time. There is no consensus on the most effective way to combat decoherence. Complex pulse sequences are necessary, but qubit analysis under such conditions is difficult, so a tool that illustrates the qubit’s evolution would be indispensable. Using the QuTip programming language, I will create a tool that searches for, visualizes, and optimizes the pulse sequences that optimize qubit coherence. Visualizing qubit evolution as an animated arrow on the Bloch sphere is a critical step towards the goal of implementing machine learning to find the pulse sequences that protect qubits against decoherence. Ultimately, this project will facilitate our understanding of the prominent decoherence mechanics in experimental platforms like spin-spin interactions and spin-lattice relaxations in solid-state spin qubits.
Modeling Interparticle Interactions in Nanocrystal Electrostatic Self-Assembly
Alexandra (Alex) Hinkle, 3rd-Year, Chemistry
Mentor(s): Prof. Dmitri Talapin, Chemistry

Self-assembly of functional nanocrystals has been used to form highly-ordered crystalline superstructures with condensed matter properties, particularly of interest for their electronic band structures. However, these nanocrystals are typically studied using bulky organic ligands for stabilization which prevent dense packing and obstruct extended electronic properties of the system. As an alternative, our approach has examined using small, anionic chalcogenidometallate ligands to better enable densely packed structures. This primarily results in electrostatic-mediated assembly, which correlates closely with the classical colloidal electrostatic stabilization mechanisms predicted by Derjaguin–Landau–Verwey–Overbeek (DLVO) theory. Here, we use DLVO theory and modified DLVO potentials to computationally model the assembly conditions for nanocrystal systems with ionic ligands. Initial results show that these models agree with the trends observed experimentally, showing that DLVO theory is an attractive method for understanding electrostatic assembly in charged nanocrystal systems. However, we also show that traditional DLVO theory alone is incomplete for fully describing nanocrystal systems, which may be due to Pauli repulsion of the ligands. As such, this model has tentatively been improved by introducing a short-distance repulsion term to account for the dynamic presence of ligands on the particle surface. Future work will focus on applying these principles to assemble various semiconducting nanocrystal systems including PbS and PbSe and to explore additional experimental conditions including ionic strength and temperature. Investigating the assembly of ionic nanocrystal systems will help to better understand the foundational mechanics behind strongly coupled nanocrystal superlattices.
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Investigating the Radial Density Distribution in Galaxy Cluster Cores
Alexandra Masegian, 2nd-Year, Astrophysics, English and Creative Writing
Mentor(s): Dr. Yuanyuan Zhang, Kavli Institute for Cosmological Physics, Fermi National Accelerator Laboratory

Understanding the radial distribution of galaxies inside galaxy clusters is necessary to place constraints on a variety of astrophysical effects and dark matter properties. Of particular importance is the distribution of galaxies in the innermost regions of clusters, where high matter densities lead to interesting interactions such as galaxy stripping and disruption that play an important role in current models of galaxy evolution. However, these cluster centers are difficult to study, as the high density of galaxies produces a blending effect that interferes with our ability to accurately recover the properties of individual cluster members. In this work, we aim to make highly accurate measurements of radial density profiles in the inner regions of galaxy clusters by applying corrections derived from Balrog, an image simulation and bias-detection approach developed within the Dark Energy Survey (DES). In this approach, simulated galaxies with known properties are injected into raw observational data of galaxy clusters. The images are then processed using the official DES reduction pipeline, and the measured properties of the simulated galaxies recovered by the pipeline are compared to the initial properties assigned by Balrog. Any discrepancies can then be used to estimate the detection efficiency and measurement biases of the DES pipeline, which are applied as corrections to measurements of real galaxy properties. Using this approach, we aim to probe the innermost regions of galaxy clusters more deeply than previous studies. The resulting cluster density profiles have the potential to provide new insights into galaxy evolution processes. By comparing our measurements to simulations of cluster evolution under different dark matter frameworks, we will be able to provide new evidence about intra-cluster interactions that until recently have been out of reach due to blending effects.
Characterizing Y$_2$O$_3$:Eu Nanoparticles for Treatment of Ovarian Cancer

Ariel Pan, 4th-Year, Chemistry & Biochemistry
Mentor(s): Prof. Chin-Tu Chen, Radiology; Jeffrey Souris, Biological Sciences Division

Often diagnosed in the late stage due to its vague symptomatology (e.g. bloating, abdominal pain) and a lack of reliable screening tests, ovarian cancer is considered the fifth deadliest cancer for women in the U.S. Although treatment usually begins with cytoreductive surgery and chemotherapy, metastatic ovarian cancer is prone to relapse and chemoresistance, making radiotherapy a common second-line treatment. However, whole abdominal radiation (WAR) is quite toxic at the necessary therapeutic levels, which can lead to serious chronic side effects that decrease patient quality of life. To counter this issue, we have developed europium-doped yttrium oxide nanoparticles (Y$_2$O$_3$:Eu NP) for use in low-energy x-ray activated photodynamic therapy (X-PDT), in which the NP produce cytotoxic reactive oxygen species (ROS) when irradiated with x-ray. The ROS production enhances the radiation treatment, allowing lower x-ray doses to be used, and thus reducing toxic side effects. This study aimed to optimize further modifications of these NP for in vivo use. To prevent NP aggregation and improve biocompatibility, a silica shell coating was added to the NP using a modified Stöber reaction. Transmission electron microscopy (TEM) was performed on samples taken at 6-, 10-, 12-, and 24-hour timepoints to monitor silica shell thickness (5-10 nm is ideal to ensure sufficient ROS production), with shorter reaction times giving more ideal NP sizes. In order to target the tumors specifically, the silica-coated NP were also conjugated with monoclonal antibody 47 (mAb47), which binds interleukin 13 receptor alpha 2 subunit (IL13Rα2), a protein overexpressed in most ovarian cancer cell lines, with high affinity. Antibody conjugation to the NP was proposed to work via a PEG-NHS linker, and fluorescence spectroscopy studies were conducted to confirm pegylation. Ultimately, these mAb47-conjugated nanoparticles will be used to conduct in vivo studies with mice to determine their efficacy.
Learning Manifolds From Point Clouds
Isabella DeClue, 2nd-Year, Statistics, Computer Science
Mentor(s): Prof. Lorenzo Orecchia, Computer Science; Ryan Robinett, Computer Science

A manifold is a mathematical space that can locally be mapped with Cartesian coordinates, but may have complex properties globally. One example of a manifold that is easy to conceptualize is a sphere, which resembles a 2-dimensional plane when one only looks at points near a fixed center. Manifolds have been widely studied in many areas of mathematics and statistics, which has led to the formation of the Manifold Hypothesis. This hypothesis states that empirical probability distributions in various sciences (e.g. the results of mRNA sequencing in Biology) tend to possess an underlying, low-dimensional structure. Reducing the dimension of complex datasets while retaining key information is an important focus of modern methods of data analysis, and the Manifold Hypothesis gives reason to believe this can always be achieved. One of the most common dimensionality reduction procedures is Principle Component Analysis (PCA), which empirically determines the best linear approximation of specified dimension to a dataset. Little et al. (2017) proposed an adaptation of PCA called multiscale Singular Value Decomposition (mSVD) that is able to recover the local Cartesian structure of point clouds with high fidelity. It is well known that local Cartesian charts like this can be “stitched together” to allow for a unified, global representation of the underlying manifold. My research over the past academic year has focused on the development of computational methods to perform this stitching via manifold triangulation. By creating a robust process for triangulating simpler and eventually more complex manifold structures, we grow one step closer to learning the global manifold representations underlying empirical point clouds.
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Statistics of Exoplanetary Resonant Chains
Jared Siegel, 3rd-Year, Physics & Astrophysics
Mentor(s): Prof. Daniel Fabrycky, Astronomy and Astrophysics

The number of detected exoplanets has boomed over the last decade. Over 4,000 planets have been confirmed, primarily by the Kepler mission, with thousands more expected from TESS and PLATO. This wave of detections has revealed an incredibly diverse population of planets and system architectures. Of particular interest are resonant chains, planetary systems containing multiple adjacent planet pairs with orbital periods near an integer ratio (2/1, 3/2, 4/3, …). These systems are a natural outcome of standard planetary formation theories and are a potential fossil record of planetary migration. Here we search for evidence that resonant pairs are correlated with one another; if so, the probability that a given planet pair is resonant is higher if an adjacent pair is resonant as well. We conduct this study using Bayesian statistics and Monte Carlo simulations. We first model the observed period ratio distribution as a smooth continuum with Gaussian spikes at the resonances. From this model, we calculate the likelihood that a given period ratio is resonant or merely part of the continuum. For each observed exoplanetary system, we then calculate the probability of forming a similar system, by random sampling of period ratios. Our preliminary results indicate there is an excess of exoplanetary systems with three or more adjacent resonances, suggesting a correlation between resonant pairs. We are now investigating whether this trend is an observational artifact, by investigating a series of prior distributions for the planet sizes, orbital periods, and inclinations.
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Molecular Latent Space Simulators: Ultra-efficient Molecular Simulations of Protein Folding and Amyloid Aggregation
Joseph (Joe) Aulicino, 3rd-Year, Mathematics & Molecular Engineering
Mentor(s): Prof. Andrew Ferguson, Pritzker School of Molecular Engineering

As computing becomes less expensive, the interdisciplinary techniques of computational biology have become salient and effective. Molecular dynamics (MD) is a computational strategy which probes physical properties by simulating the movements of atoms. MD and other bioinformatics techniques can address properties about a system of interest more easily than physical experimentation. Computational simulation is typically more cost efficient than physical experimentation and allows for high-throughput virtual screening to facilitate expedited drug discovery and molecular engineering. While improvements in algorithms have allowed for the simulation of complex billion atom systems, increases in the length of simulated time have proven elusive. Presently, MD techniques are limited to microsecond timescales on commercially available processors. This means key rare events (e.g., enzyme docking, protein folding, protein aggregation), are sampled rarely and have high uncertainties. Thus, advancing the length of simulated time, the “time-scale barrier,” is of key research importance. In this work, I evaluate the Latent Space Simulators approach (LSS), first formalized by the Ferguson Lab in August 2020. LSS is a machine learning approach that learns a kinetic model over the limited MD training data, which enables the observation of rare states like protein folding, enzyme docking, and protein aggregation. LSS represents an enabling technology to simulate the kinetic behavior and properties of large molecular systems of biological relevance that are currently outside the reach of existing computational approaches.
Banded Vegetation Patterns in Drylands: Modeling Across Timescales
Lily Liu, 4th-Year, Mathematics
Mentor(s): Prof. Mary Silber, Computational and Applied Mathematics, Punit Gandhi, Mathematics and Applied Mathematics, Virginia Commonwealth University

Periodic spatial patterns of vegetation growth have been observed in dryland ecosystems. These patterns are thought to arise through self-organization in the water-limited environments that support them, and reaction-advection-diffusion models have suggested that the patterns are a precursor to ecosystem collapse as water becomes increasingly scarce. On gently sloped terrain, dryland vegetation patterns often appear as repeating bands of dense vegetation that are decameters wide and spaced on the order of hectometers apart, with bare soil in between. While observations indicate uphill migration of the bands on a century timescale, the water is input during rainstorms that last just a few hours. We explore the impact of assumptions about the fast hydrology associated with overland flow and infiltration during rainstorms on the slow dynamics of the patterns. We consider both temporally periodic and stochastic rain input within a conceptual fast-slow switching model that exploits the difference in timescales involved.
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**Theory of Bipolarons in Strontium Titanate (SrTiO₃)**
Lisa Lin, 4th-Year, Physics
Mentor(s): Prof. Peter Littlewood, Physics

The origin of superconductivity in the doped semiconductor strontium titanate (STO) is not well-understood. Its persistence even at very low carrier densities violates key assumptions of conventional Bardeen-Cooper-Schrieffer (BCS) theory, particularly in that the phonons in this regime are much faster than the electrons to which they are coupled. The formation of bipolarons, two-electron bound states in a polar medium, serves as a potential electron pairing mechanism beyond the BCS paradigm. Here, the existence of bipolarons in STO is probed using semiclassical analyses and variational calculations to estimate the system’s ground state energy in the weak- and strong-coupling limits of the electron-phonon interaction strength in STO, respectively. It is found that no binding exists in the weak-coupling regime, whereas the strong-coupling regime exhibits strong binding. We explore the intermediate regime through Quantum Monte Carlo (QMC) simulations, which enable exact calculation of the ground state energy.
Galaxy-Galaxy Lensing of Low-Surface Brightness Galaxies
Nathalie Chicoine, 2nd-Year, Astrophysics & English
Mentor(s): Prof. Chihway Chang, Astrophysics; Dr. Judit Prat, Astrophysics, Chang Lab

Massive objects create gravitational wells that warp the path of light. When the light of background (source) galaxies passes close to foreground (lens or tracer) galaxies, it gets perturbed, distorting the image of the source galaxies we receive. We can measure this distortion, known as gravitational lensing shear, to estimate the mass of objects not visible to other techniques. In the case of a spherical distribution of matter, the shear at any point will be oriented tangentially to the direction of the center of symmetry. Due to the random intrinsic orientation of galaxies, this distortion of galaxy shapes is rarely noticeable or measurable for a single object. To obtain a signal, we must average the tangential component of the shear over many lens-source galaxy pairs. For our research, we performed this measurement, called galaxy-galaxy lensing, to obtain the tangential shear profiles of low-surface brightness galaxies: faint, diffuse galaxies composed primarily of non-baryonic matter or dark matter. Owing to their dimness, we know little about the structure or formation of these galaxies. Our next steps include fitting these shear measurements with a Halo Occupation Model (HOD) to profile the dark-matter make-up of these galaxies and measure their mean halo mass.
Formation and Persistence of Ice Rumplers
Niall Coffey, 4th-Year, Physics & Economics
Mentor(s): Prof. Douglas MacAyeal, Geophysical Sciences

One of the most striking features of Ellesmere Island Ice Shelves is the rolling surface topography, known as ice rumplers. However, the mechanisms governing how these sinusoidal surfaces arise, as well as how these features persist, have not fully been tested. In this research, we seek to test which natural forcings could initiate and maintain ice rumplers through numerical modeling and theoretical analyses. Identifying the dominant forcings and associated time and pressure scales in formation and persistence is important groundwork for understanding ice shelf stability, where mass flux and ice shelf ablation directly contribute to global mean sea level.
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**Developing and Exploring Computational Tools in Python and MySQL to Decode Inca Khipus**

Nyaga Kariuki, 2nd-Year, Mathematics, Religious Studies

Mentor(s): Prof. Jon Clindaniel, Computational Social Science

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Many tools have been created to analyze various representational systems; the Inca Khipus present unique opportunities by virtue of being a knot-cord system. Khipus were one of the primary communication methods of the pre-Hispanic Inca Empire. Until now, we have understood their numerical codes. The research of Gary Urton has shown the majority of patterns on Khipus contain numerical information, however we still need to decode non-numerical patterns and fully analyze the patterns contained in the numbered parts. Under Dr. Jon Clindaniel, I have worked to analyze Khipu data and create resources for other researchers. Throughout the process, I have incorporated social scientific and qualitative studies from people such as Gary Urton and Marcia and Robert Ascher. Using the Open Khipu Research Laboratory data, I have modified a number pattern recognition code from Dr. Clindaniel’s thesis to work for colors, knot types, and other descriptive elements of the Khipus. Furthermore, I have prepped the Open Khipu Research Laboratory Github for use by both technical and non-technical parties. In the presentation, I will discuss these advances and how they will be used both by me and other researchers to continue investigating questions on the Inca Khipu system.
Are Machine Learning Cloud APIs Used Correctly?
Shicheng Liu, 3rd-Year, Computer Science & Mathematics, Physics
Mentor(s): Prof. Shan Lu, Computer Science

Recent years have witnessed rapid advancement of machine learning (ML) technologies. Speech recognition, medical diagnosis, smart assistants, self-driving cars, and many more technologies backed by ML are drastically transforming our lives. In particular, numerous cloud service providers (e.g. Google Cloud and Amazon Web Service) have developed a range of machine learning products that market on their accessibility to software developers. These ML application programming interfaces (APIs) enable developers to easily incorporate machine learning solutions into software systems. Unfortunately, ML APIs are challenging to use correctly and efficiently, given their unique semantics, data requirements, and accuracy-performance tradeoffs. Much prior work has studied how to develop ML APIs or ML cloud services, but not how software applications are using ML APIs. We present the first in-depth study of real world applications using ML cloud APIs. We manually study 360 representative open-source applications that use Google or Amazon AWS cloud-based ML APIs, and identify 70% of these applications as containing API misuses in their latest versions that degrade functional, performance, or economical quality of the software. These misuses lead to various types of problems, including 1) reduced functionality, such as a crash or a quality-reduced output; or 2) degraded performance, like an unnecessarily extended interaction latency; or 3) increased cost, in terms of payment for cloud services. Their root causes are all related to unique challenges for ML APIs. We have generalized 8 anti-patterns based on our manual study and designed several checkers and small API changes (in the form of wrapper functions) that both check for and handle common errors. Hundreds of more applications are identified as containing misuses by our checkers, beyond the 360 projects in the initial study.