UNIVERSITY OF DELAWARE
DATA SCIENCE INSTITUTE

DELAWARE Data Science

DARWIN COMPUTING SYMPOSIUM

FEB 23, 2023

#DARWINcomputing2023

Agenda

Registration and Poster Setup	8:30 – 9:00 AM
Introduction – Welcome Remarks: Marianna Safronova, Committee Chair	9:00AM
Remarks from Laura Carlson, UD Provost	9:15AM
Remarks from Varun Chandola, NSF-AOC	9:30AM
Session I – Science on DARWIN	9:45AM
Coffee Break	10:45AM
Session II – Broadening Participation: Regional/National Resources	11:00AM
Lunch	12:00 PM
Poster Lightning Talks	12:40PM
Poster Session	1:15PM
Session III – Science on DARWIN: The Next Generation	2:20PM
Session IV – HPC and Data Science: Current and Future Initiatives	3:20PM
Coffee Break	4:00PM
Panel: What is next?	4:15PM
Best Poster Award & Closing Remarks	4:55PM

WELCOME REMARKS

Marianna Safronova

Chair DARWIN Computing Symposium Planning Committee
Professor, Physics & Astronomy
University of Delaware

REMARKS FROM UD PROVOST

Laura Carlson

Provost
University of Delaware

REMARKS FROM THE NSF

Varun Chandola

Office Director, Office of Advanced Cyberinfrastructure (OAC) , National Science Foundation

“Building a Sustainable Scientific Cyberinfrastructure Ecosystem”

I will briefly introduce the initiatives at the National Science Foundation (NSF), and specifically within the Office of Advanced Cyberinfrastructure (OAC), towards realizing the vision for a sustainable scientific cyberinfrastructure ecosystem, which includes investments for hardware, software and data, services, and learning and workforce development. I will also briefly describe some of the upcoming funding opportunities at NSF that might be of interest to the audience.

SESSION I

SCIENCE ON DARWIN

Cathy Wu *(Moderator)*

DARWIN co-PI
Director, Data Science Institute
University of Delaware
https://dsi.udel.edu/

Krzysztof Szalewicz

Professor
Physics & Astronomy
University of Delaware
https://www.physics.udel.edu/people/szalewic

"Computational Predictions of Properties of Materials Without Any recourse to Experimental Information"

Abstract: It is now possible to numerically solve the equations of quantum mechanics for molecules consisting of hundreds of atoms and predict macroscopic properties of matter with high precision. The whole procedure does not use any experimental information on the investigated systems, yet such theoretical predictions "from first principles" can agree very well with available experimental data. For example, it is possible to predict from first principles the boiling temperature of water and the melting temperature of ice. While these properties are, of course, well known from experiments, some regions of the water temperature versus pressure diagram are not accessible experimentally and remain unknown. Another example are predictions of crystal structures. A given molecule can crystallize in tens of thousands plausible structures, but only a couple of them, in most cases just one, can be found experimentally. It is now possible to predict which form will be found using first-principles approaches. Such predictions are of significant importance for pharmaceutical, energetic materials, and other industries. Some algorithmic and programming developments making such work possible will be outlined.

Anderson Janotti

AssociateProfessor
Materials Science & Engineering
University of Delaware
https://mseg.udel.edu/people/janotti/

“Discovery and Characterization of Electronic and Quantum Materials Through Computation”

Advances in parallel computation and algorithm implementation have enabled accurate quantum mechanical descriptions of materials systems with hundreds of atoms and thousands of electrons. Electronic structure methods based on the density functional theory with periodic boundary conditions become the workhorse in the simulations of defects in semiconductors, interfaces, and surfaces. In this presentation, we use examples from our own research group to describe how we employ these advanced computational methods in the discovery of new materials and new phenomena in materials science and help guide experimental efforts in the characterization of existing materials. We discuss exotic types of hydrogen bonding in oxides, qubits derived from single defects in semiconductors and insulators, interfaces of quantum materials, interfacial two-dimensional electron or hole gases, embedded nanoparticles in semiconductor matrices, and other interesting interface and surface phenomena. These examples serve to illustrate the instrumental role DARWIN has been playing in our current research.

Rodrigo Vargas

Professor
Plant & Soil Sciences
University of Delaware
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“Environmental Data Science to Address Global Grand Challenges”

Environmental data science plays a crucial role in addressing global grand challenges. Some of these grand challenges include climate change, water scarcity, and land use change, among others. With increasing data available from multiple sources, it is now possible to develop models and multidisciplinary approaches to help us better understand the underlying processes that drive these grand challenges. Multiple efforts associated with environmental data science exist across colleges at the University of Delaware. This presentation will highlight efforts that use computing resources to analyze large volumes of data across Delaware, the United States, and the world. Examples include analysis of soil moisture, changes in vegetation dynamics, and land use changes. Faculty at UD leverage the power of data and technology to gain a deeper understanding of the natural environment, identify the most pressing problems, and design solutions.

SESSION II - BROADENING PARTICIPATION: REGIONAL/NATIONAL RESOURCES

Benjamin Bagozzi *(Moderator)*
DARWIN co-PI
Associate Professor
Department of Political Science & International Relations
University of Delaware
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Cherese Winstead
Dean of the College of Agriculture, Science and Technology (CAST)
Professor, Department of Chemistry
Delaware State University
https://cast.desu.edu/about/faculty-profiles/cherese-winstead-phd

“Ensuring Broadening Participation and Engagement in Data Science”

Broadening participation in data science takes on diversity of perspectives in terms of race, gender, socioeconomic status, ethnicity, and first-generation status, which ultimately creates the foundation for the transdisciplinary nature of the field. One of the challenges facing the inclusion and engagement of URMs in data science is bridging the gap between access, education and application. Inclusive environments must be fostered to ensure that students and faculty have equitable access to resources (e.g., high-quality data, tools, technology, adaptable and appropriate curriculum, and advisors). It is essential that attraction and engagement of URMs in data science employ problem solving using real-world examples, to mediate and moderate STEM persistence and success. It is also imperative that URMs are supported both financially, academically and through mentorship, to fully recognize the opportunities that the field of data science presents and the value they can add to it. Lastly, the multidisciplinary strength of data science should serve as an ideal vehicle to improve broadening participation in STEM to address next generation concerns such as social and environmental justice, health disparities and policy changes, thereby helping to increase enrollment of minorities and women in STEM. Overall, ensuring broad participation in data science should have the elements of “culturally relevant curricula,” diverse faculty, shared resources and equitable collaborations between majority- serving and minority-serving institutions to fulfill our future workforce needs and to improve the quality of tomorrow’s solutions.

Anita Schwartz

Lead Scientific Application Consultant, HPC Team
University of Delaware

"ACCESS: Building on XSEDE's Success"

The NSF's ACCESS (Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support) program builds upon the successes of the 11-year XSEDE (Extreme Science and Engineering Discovery Environment) project, while also expanding the CI (cyberinfrastructure) ecosystem with capabilities for new modes of research and further democratizing participation. This presentation highlights ACCESS Services, how to get started with ACCESS and how it differs from XSEDE.

Juan Perilla

Assistant Professor
Chemistry & Biochemistry
University of Delaware
http://biophysics.chem.udel.edu

"Discovery Through the Lens of the Computational Microscope"

The essential conundrum of modern biology, namely the question of how life emerges from myriad molecules whose behavior is governed by physical law alone, is embodied within a single cell—the quantum of life. The rise of scientific supercomputing has allowed for the study of the living cell in unparalleled detail, from the scale of the atom to a whole organism and at all levels in between. In particular, the past three decades have witnessed the evolution of molecular dynamics (MD) simulations as a "computational microscope", which has provided a unique framework for the study of the phenomena of cell biology in atomic (or near-atomic) detail. Our work synergistically combines single-molecule biophysics, structural biology and computational biology techniques to probe the molecular origin of biological phenomena. Here I present an overview of our synergistic efforts with experimentalists to determine the molecular details during the life-cycle of HIV-1. Our work reveals complex relationships between capsid permeability and reverse-transcription, and deciphers the role of host-factors during the life-cycle of the virus.

Michael Blaustein
Industry Liaison, Data Science Institute
University of Delaware

"Corporate Engagement"

Opportunities and approaches for private sector engagement with the Data Science Institute and DARWIN will be presented.

SESSION III

SCIENCE ON DARWIN: THE NEXT GENERATION

Rudolf Eigenmann *(Moderator)*
DARWIN Principal Investigator (PI)
Director, Data Intensive & Computational Science (DICoS) Core
Professor, Electrical and Computer Engineering
University of Delaware
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Manju Anandakrishnan
PhD Student, Bioinformatics Data Science
Wu Lab
University of Delaware

"KSFinder – A Knowledge graph Embedding and Deep Learning Tool for Predicting Protein Phosphorylation"

The majority of the computational tools for studying phosphorylation utilize local feature selection techniques on the basis of protein motifs, domains, sequences, functions, or a combination of these. These tools fail to consider the heterogeneous relationships of the proteins in context with multiple biological entities, which is an inherent mechanism in cellular processes. Moreover, the existing tools have limited kinase coverage. Though there are 512 known human kinases, most of the existing tools scope their study to less than 50% of the human kinases. In this study, we built a predictive modeling tool, KSFinder developed using a dataset that includes 467 kinases and their protein substrates. The model incorporates a two-step approach integrating graph embedding and supervised deep learning. Initially, the semantic relationships among the entities in the biological network are learned using the knowledge graph embedding (KGE) algorithm and represented in a low-dimensional vector. Then, the embedded vectors of the kinases and substrates are extracted and utilized as features to train a neural network-based multi-layer perceptron (MLP) classifier model. The performance of KSFinder surpassed the two other KGE-based phosphorylation prediction models, LinkPhinder and TripleWalk, with an AU- ROC of 0.852. KSFinder predicted 281 substrates for the understudied kinase, NUAK family SNF1-like kinase 2 (NUAK2) with a probability over 0.75. The manual review of the literature showed experimental evidence of NUAK2 phosphorylating two of our predicted substrates – MYPT1 (Protein phosphatase 1 regulatory subunit 12A) and MLC2 (Myosin regulatory light polypeptide 9). The prediction probabilities of these substrates are 0.79 and 0.84 respectively. Enrichment analysis of the predicted substrates provides clues for the protein being involved in stress-induced cellular processes, cell cycle, and apoptotic signaling due to viral stimulus, and oxidative stress. Though the kinase has been previously annotated for being involved in apoptosis, our analysis hints at its participation in stress-induced apoptosis. Knowledge graph embedding of large datasets requires GPU resources that can leverage multiple cores. Our dataset contained approximately 1 million triples and we trained four graph embedding models using the scoring functions – ComplEx, DistMult, TransE, and HolE along with different hyperparameter values to determine the optimal model for embedding our data. We leveraged the high-performance computing (HPC) cluster – DARWIN for GPU resources. Specifically, the compute nodes - nVidia-V100, and nVidia-T4 on the cluster were utilized in addition to the GPU resources in our lab. In order to take advantage of the GPU resources, a custom conda environment was created and the libraries - tensorflow-gpu, NVIDIA's CUDA toolkits, and Ampligraph were installed. A VALET package definition was created, and the custom environment was configured. We then loaded this VALET package to train our embedding and MLP model. Approximately, we utilized 2 nVidia-V100 GPUs for 60 minutes and trained the graph embedding model with a dataset of size 1 million relations; 1 nVidia-T4 resource for 12 minutes to perform hyperparameter optimization and trained a multi-layer perceptron model with 10-fold cross-validation on a dataset of about 10,000 records.

Ankit Kulshrestha
PhD Student, Computer & Information Science
Safro Lab
University of Delaware

"Avoiding Barren Plateaus in Variational Quantum Algorithms"

In the current NISQ regime of Quantum Computing, Variational Quantum Algorithms (VQAs) are one of the most promising areas that have the potential of demonstrating a "quantum supremacy". These algorithms solve different optimization problems using parameterized quantum circuits whose parameters are optimized on a classical computer using a classical optimization algorithm. The optimal parameters correspond to a quantum state which when measured produces a minima (maxima) of the objective function. However, these circuits currently suffer from a notorious barren plateau problem - they have a tendency to get stuck in suboptimal regions of the optimization surface even when the depth of circuit is at most polynomial. In this talk we discuss the issue and present a solution to help quantum circuits avoid such plateaus.

Chris Lashley

Postdoctoral Researcher
Center for Applied Coastal Research
University of Delaware

"Contribution of Wave Runup to Coastal Flooding at Norfolk during Hurricane Irene"

Coastal flooding occurs when the total water level (TWL) exceeds that of the natural (e.g., dune) or built (e.g., levee) coastal defense. Operational models used to forecast TWL's typically consider the combined effect of mean sea level, high tide, and storm surge. However, the extent to which storm waves runup the beach or structure is often neglected, as computationally demanding numerical models are typically needed to resolve the individual waves. Despite being more practical, several studies suggest that excluding wave runup can lead to a significant underestimation in the resulting coastal flooding. Here, we assess the contribution of wave runup to coastal flooding at Norfolk (VA, USA) during Hurricane Irene (2011) using the FUNWAVE numerical model—made feasible thanks to the DARWIN high performance computing system.

SESSION IV - HPC AND DATA SCIENCE: CURRENT AND FUTURE INITIATIVES

Marianna Safronova (Moderator)

Chair DARWIN Computing Symposium Planning Committee
Professor, Physics & Astronomy
University of Delaware

Rudolf Eigenmann

DARWIN Principal Investigator (PI)
Director, Data Intensive & Computational Science (DICoS) Core
Professor, Electrical and Computer Engineering
University of Delaware

"Computing Projects and Initiatives at the University of Delaware"

This talk provides an overview of computational and data science projects and initiatives at the University of Delaware. Initiatives that complement computational thrusts will also be summarized. Today, computational research spans nearly all UD colleges and many of their departments. While the DARWIN machine is a key enabler, the talk will also describe other resources, both at UD and nationally, that support the research projects.

John Huffman

Director
IT Research Cyberinfrastructure
University of Delaware

"HPC at UD: Where We Are, and What Comes Next"

An overview of the current state of HPC at the University of Delaware and how it is being utilized. We will also look at some of the challenges and opportunities we and other research institutions face as technology continues to evolve.

PANEL DISCUSSION: TALK ABOUT THE FUTURE

Rodrigo Vargas *(Moderator)*

Professor
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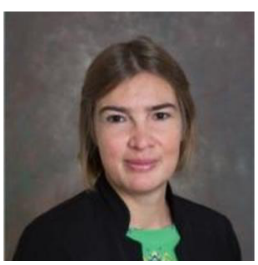
Kelvin Lee

Interim Vice President for Research, Scholarship and Innovation
Director, National Institute for Innovation in Manufacturing Biopharmaceuticals (NIIMBL)
Gore Professor Of Chemical & Biomolecular Engineering
University of Delaware

Rudolf Eigenmann

DARWIN Principal Investigator (PI)
Director, Data Intensive & Computational Science (DICoS) Core
Professor, Electrical and Computer Engineering
University of Delaware



Marianna Safronova

Chair DARWIN Computing Symposium Planning Committee
Professor, Physics & Astronomy
University of Delaware

John Huffman

Director
IT Research Cyberinfrastructure
University of Delaware

POSTER SESSION

1. **James Korman, PhD Student, Political Science & International Relations, University of Delaware**
*Title***:** Assessing The Impact of Wealth Inequality on State Capture in Latin America
Abstract: Economic inequalities are the defining issues of our time. This paper presents the first empirical study using a novel variable Top 1% share wealth inequality derived from the World Inequality Database that directly measures the top 1%'s share of wealth overall. The study examines the empirical effect of the top 1 percent's share of wealth inequality in contributing to state capture. 19 Latin American countries are analyzed across the temporal period 1996-2021. A random effects regression model is used enabling the exploitation of between level variation to greater generalize the results across the Latin American region while minimizing bias to the coefficient estimates. The results demonstrate that top 1% wealth inequality is highly statistically significant and positive in explaining the variation in state capture. The greater the share of wealth the 1% hold, the more state capture we should expect.
2. **Katie Raudenbush, PhD Student, Chemical & Biomolecular Engineering, University of Delaware**
Title: Predicting the effects of gradients on cell culture performance in large scale bioreactors
Abstract: Monoclonal antibodies (mAbs) are a major class of biotherapeutics, treating cancers, autoimmune diseases, and even COVID-19. Scale-up of bioreactors is necessary for industrialization of monoclonal antibody (mAb) production but can lead to the formation of spatial gradients in important culture parameters such as dissolved oxygen. These gradients can have adverse effects on cell culture dynamics including lower cell density, productivity, and product quality. In-silico modeling enables us to predict the presence and effects of spatial gradients in large scale bioreactors. Unsteady computational fluid dynamics (CFD) is performed to predict dissolved oxygen concentrations spatially in the bioreactor and to track 'lifelines' of cells' exposure to these heterogeneities. These 'lifelines' are then coupled to a kinetic model of cell metabolism to predict the impact of oscillating dissolved oxygen on a full 14 day cell culture with mAb production.
3. **Antoine Mathieu, Postdoctoral Researcher, Civil & Environmental Engineering, University of Delaware**
Title: Investigation of bedform formation using an Eulerian two-phase model
Abstract: A full understanding of the mechanisms responsible for bedform formation is not yet achieved. In this work, we propose a new tool to investigate the formation of ripples starting from an initially flat bed: the Eulerian turbulence-resolving two-phase model. An experimental configuration is reproduced numerically and numerical experiments are performed to assess the predictive capabilities of the two-phase model. Even if the results show a grid-size dependency, the main features of ripple formation are reproduced by the model. We show that the Eulerian two-phase model can be a great tool to investigate bedform formation, especially to investigate the role played by small scale turbulent structures in the early stage of ripple formation.
4. **Juan Rey, PhD Student, Chemistry & Biochemistry, University of Delaware**
Title: Deriving the structure of HIV-1 immature Gag lattice at multiple scales
Abstract: HIV-1 Gag constitutes the building block of the immature virion. Although it has been studied extensively as a drug target for maturation inhibition, there is yet no public structure available of a fully atomistic immature HIV-1 capsid. Here, we present a procedure for deriving fully atomistic viral lattices from cryo-EM tomograms by combining image processing techniques and molecular simulation. We apply our method to the immature HIV-1 Gag, generating a quasi-spherical lattice that conserves the interhexamer and intrahexamer CA interfaces as well as allowing us to characterize the gap distribution and curvature of the native viral capsid. Furthermore, we explore reducing the number of degrees of freedom of the simulation system by performing shape based coarse graining on the CASP1 monomer. Our SBCG model reproduces the atomic structure to sub nanometer resolution, while reducing the atom count by an order of magnitude.
5. **Manan Sarupria, PhD Student, Geography, University of Delaware**
Title: Spectral unmixing of satellite images for quantifying salt-impacted farmlands in Delmarva.
Abstract: Saltwater intrusion (SWI), the inland encroachment of saltwater into freshwater aquifers, in coastal areas, is mainly driven by sea level rise, storm surge, and excess groundwater pumping. Collecting field-level data on soil salinity can provide an accurate measure of the extent of salinization, but it is challenging to scale up to geographically larger regions. We aim to use advanced machine learning techniques to capture the spatial distribution of salt patches on the soil surface across 14 coastal counties in the eastern USA states of Delaware, Maryland and Virginia. While high-resolution aerial images can be used to quantify the extent of these fine-scale salt patches, these images do not have high temporal resolution. Our objective is to derive annual maps of salt-impacted lands to better aid landowners' decision-making process. The resulting images will contain each pixel with a fraction value corresponding to the percentage of pixel area covered by salt patch.
6. **Matthew Walter, PhD Student, Geography, University of Delaware**
Title: Topic modeling and satellite data for identifying environmental injustice in Philadelphia
Abstract: Prior research has quantified the characteristics of parks and uncovered that park quality in the USA may not be equally distributed, with lower quality parks being associated with vulnerable groups, lowering the benefits they receive from parks. While these studies identify injustice, they do not consider the voices of those being impacted by urban park quality. Rather than basing quality on a park's physical

characteristics, we let park users speak for themselves by measuring the public perception of 285 Philadelphia parks across 143,913 Google reviews. We conduct an analysis to identify parks that are accessible to a range of vulnerable groups and the Google review score of those parks. Google review texts are summarized using anchor word-assisted topic modeling to gauge the factors affecting park perception. Results allow practitioners to identify the demographic groups and geographic areas that are associated with negative park perception and the drivers behind the disparity.

7. **Kelsey Edwing, Master's Student, Marine Science, University of Delaware**
   Title: Impact of Marine Heatwaves on Air-Sea CO2 Flux in the Northwest Atlantic Margins
   Abstract: Marine heatwaves (MHW) are extreme sea surface temperature events that have the potential to impact air-sea CO2 fluxes. However, this concept has not been explored in the nearshore waters of continental shelves. Understanding how coastal air-sea CO2 fluxes (FCO2) are modulated by MHW events is important for furthering our comprehension of coastal biogeochemical cycles and for improving predictions of future climate change impacts. As such, this study quantifies the influence of MHWs on FCO2 in Mid Atlantic Bight (MAB) and South Atlantic Bight (SAB) and determines the driving mechanism(s). To achieve this, we use a case study of the longest MHW event in each region to examine the mechanism(s) controlling the ensemble average of all MHW events in each region. Results thus far have indicated that the thermal influence of MHW events induce positive FCO2 anomalies, reducing each region's ability to act as CO2 sinks by lowering CO2 uptake and increasing outgassing.
8. **Deanna Edwing, Master's Student, Marine Science, University of Delaware**
   Title: Characterizing Delaware Bay Coastal Flooding using Sentinel-1 SAR Imagery and Machine Learning
   Abstract: Flooding is among the most common yet costly world-wide annual disasters. With climate change modifying local environments, coastal communities are increasingly vulnerable to flooding. In particular, Delaware is at high risk due to its flat topography, low mean elevation, and high land subsidence rates. This, combined with rising sea levels and increased storm activity, are prompting questions about coastal flooding frequency and intensity, which have increased in recent years. This study investigates coastal flooding around the Delaware Bay using Sentinel-1 SAR imagery and a neural network trained in water segmentation. The resulting flood maps, combined with ancillary geospatial and oceanographic data aid in identifying flooding hotspots, and their potential mechanisms. Results of this study indicate that coastal flooding primarily occurs in tidal marshes toward the southern part of the bay, while agricultural regions present high moisture environments following rainfall events.
9. **Lauren Olsen, PhD Student, Computer & Information Sciences, University of Delaware**
   Title: Towards Improving Visual Question Answering (VQA) for People with Visual Impairments
   Abstract: VQA is a vision and language machine learning task that attempts to generate an answer to a question based on the information in a corresponding image. Recent research demonstrates VQA's potential use translating visual information to text for people with visual impairments. However, this research also demonstrates that photos from people with visual impairments present unique challenges, such as image quality issues, to machine learning systems. Image quality issues may make it difficult for machine learning systems to recognize image content, leading to generic responses like "unanswerable". Prior research indicates that this can be a point of frustration for people with visual impairments using accessible applications, requiring extra time and effort to figure out what is going wrong and get an answer. Our research investigates how machine learning and computer vision can be used to predict the types of quality issues present in images and mitigate their impacts of VQA systems.
10. **Van Huong Le, Postdoctoral Researcher, Agriculture & Natural Resources, University of Delaware**
    Title: Optimal monitoring sites based on suLHS to improve the representativeness of global soil properties
    Abstract: We present a data-driven method for identifying optimized samples from spatial information of environmental data. The spatial univariate Latin Hypercube Sampling (suLHS), combines a Latin Hypercube to obtain a representative sample of the univariate probability distribution function and an autocorrelation model to ensure a reproducible spatial dependency function. The suLHS is tested with a case study using data of global soil respiration map that are relevant for carbon cycle science. The results show that the suLHS is able to reproduce the univariate probability distribution and the spatial variability of the global soil respiration.
11. **Joao Pereira, PhD Student, Chemistry & Biochemistry University of Delaware**
    Title: High-performance molecular dynamics of virus simulation on DARWIN
    Abstract: Elucidating large biomolecules' structural and dynamic signatures is essential to comprehend their functions. Advancements in experimental structural biology have enabled the resolution of large and complex biological structures, further enabling their study with molecular dynamics. Here, we seek to overcome the problem of scale and simulate two HIV-1 capsid topologies in explicit solvent, including 8,000,000 and 76,000,000 atoms, using cutting-edge hardware from DARWIN. We use NAMD 2.x and NAMD 3.x to show the implementation of the scalable NAMD molecular dynamics engine employing both heterogeneous and entirely GPU-resident paradigms. We demonstrate how systems that fit inside the GPU memory restriction are amenable to appreciable speedups over CPU-only deployment. Altogether, the results of our performance scaling analyses provide practical guidelines for others wishing to employ DARWIN for large-scale biomolecular simulation.
12. **Alex Bryer, PhD Student, Chemistry & Biochemistry, University of Delaware**
    Title: The HIV-1 Capsid's Mechanical Properties Facilitate Nuclear Import
    Abstract: MD simulations of viral capsids provide opportunities for high spatial and temporal resolution analysis of their mechanical properties, which may be validated against experimental analyses such as Atomic Force Microscopy (AFM). The scale of viral capsids, however, poses

challenges for MD simulation, particularly simulation of AFM experiments which far exceed accessible timescales. The technique of coarse graining has been utilized as a means to reduce atomic complexity, conferring the feasibility of simulated AFM experiments. Utilizing cryoEM data from collaborators, we constructed a native conical capsid via topology-representing coarse graining and show that model parameters such as those describing bond and angle stiffness are adept at representing the atomistic model. With a series of in silico AFM simulations, probing different regions of the conical capsid, we reveal that the HIV-1 capsid is a robust and elastic container, well-suited for intact passage through the nuclear pore.

13. **Akshay Bhosale, PhD Student. Electrical & Computer Engineering, University of Delaware**
Title: Cetus 2.0: A Tool for Automatic Parallelization of C Programs
Abstract: This poster presents an overview and evaluation of the existing and newly added analysis and transformation techniques in the Cetus source-to-source compiler infrastructure. Cetus is used for research on compiler optimizations for multi-cores with an emphasis on automatic parallelization. The compiler has gone through several iterations of benchmark studies and implementations of those techniques that could improve the parallel performance of these programs. This work seeks to measure the impact of the existing Cetus techniques on the newer versions of some of these benchmarks. In addition, we describe and evaluate the recent advances made in Cetus, which are a capability for analyzing subscripted subscripts and a feature for interactive parallelization. Cetus started as a class project in the 1990s and grew with support from Purdue University and from the National Science Foundation (NSF), as well as through countless volunteer projects by enthusiastic students.

14. **Benjamin Tsai, PhD Student, civil & Environmental Engineering, University of Delaware**
Title: An Eulerian two-phase model investigation on wave-induced scour around a single pile
Abstract: A three-dimensional Eulerian-Eulerian two-phase flow solver, SedFoam has been been proven to successfully model sediment transport under oscillatory flows in sheet flow and bedforms modes with a Reynolds-averaged Navier–Stokes (RANS) formulation. Recently, the large-eddy simulation (LES) approach has been added into SedFoam. In this study, we apply SedFoam on three-dimensional wave-induced local scour around a single vertical circular cylinder. The numerical results show both RANS and LES can resolve lee-wake vortex, yet the vortex is weaker in RANS. Comparing with the LES, RANS fails to predict strong enough horseshoe vortex which leads to underestimation of scour hole development. Although the scour depth develops at very similar rate in the early stage, RANS quickly reaches equilibrium while LES follows the experimental trend. The results show that a turbulent resolving model, LES is needed for simulating scour around structures.

15. **Carolina Perez-Segura, PhD Student, Chemistry & Biochemistry, University of Delaware**
Title: Mechanistic insights into the CpAM-induced disruption of the HBV capsid revealed by MD simulations
Abstract: Hepatitis B virus (HBV) increases the risk of developing hepatocellular carcinoma and cirrhosis. Although there is an effective vaccine for HBV, no definitive cure has been discovered. The HBV capsid – a protein shell, predominantly found with T=4 icosahedral arrangement of 120 dimeric core protein (Cp) subunits – is a promising drug target, owing to the multiple function roles it carries out during the viral lifecycle. HBV capsid assembly can be disrupted and misdirected by small molecules called core protein allosteric modulators (CpAMs). Here, we perform all-atom molecular dynamics (MD) simulations of intact CpAM-bound HBV capsids to investigate the mechanisms by which two classes of CpAMs (HAPs and PPAs) disrupt capsid structure, dynamics, and assembly. This work is pertinent for the development and optimization of new small molecule therapeutics that target the capsid of HBV..

16. **Rasanjali Ranawaka, PhD Student, Chemistry & Biochemistry, University of Delaware**
Title: Molecular determinants of HBV capsid protein recognition by nuclear-cytoplasmic exportin CRM1
Abstract: Hepatitis B virus (HBV) is a human pathogen causing vaccine-preventable liver infection where over 250 million people live with a chronic ailment. A promising target for new HBV therapeutics is the capsid, an icosahedral shell that assembles from 120-core protein (Cp) dimers to package the genome. Recent studies reveal that Cp contains nuclear export signals (NES) in its spike domain, which are recognized by chromosomal region maintenance 1 (CRM1/Exportin 1). According to experiments, Cp export from the nucleus requires CRM1, and immature HBV particles can pass intact through the nuclear pore in a CRM1-dependent manner. However, the molecular determinants of Cp recognition by the CRM1 are yet to elucidate. We employ computational modeling and molecular dynamics (MD) simulations to establish the mechanism by which the spike NES becomes exposed and adopts conformations recognizable by CRM1 with an atomistic model of the intact HBV capsid bound to the CRM1 biological assembly.

17. **Nolan Baker, Undergraduate Student, Electrical & Computer Engineering, University of Delaware**
Aaron Jarmusch, Undergraduate Student, Electrical & Computer Engineering, University of Delaware
Title: Validation and Verification of OpenMP Offloading and OpenACC Compilers on the DARWIN System
Abstract: The OpenMP and OpenACC language specifications continue to evolve, and with each new release, new features are introduced. The need to validate and verify these new features is crucial. The SOLLVE OpenMP Validation and Verification team focuses on evaluating the conformity and implementation progress of various compiler vendors across the 4.5, 5.0, and 5.1 versions of the specification. The OpenACC Validation and Verification team has created a validation testsuite to verify the OpenACC implementations across various compilers including GNU GCC, Nvidia HPC SDK, and Clacc/LLVM, using an infrastructure for a more streamlined execution. This validation and verification process is being run on the DARWIN system. The results of the testsuites' execution will be analyzed and discussed, with a focus on future developments..

18. Inbok Yea, PhD Student, Physics & Astronomy, University of Delaware

Title: GPI Observation of the Debris Disk HD 15115

Abstract: Debris disk morphology provides information about the dynamical environment of circumstellar dust. Asymmetry and other shape distortions can signal that the disk is interacting with the ISM or being stirred by nearby planets. For this study, we analyzed GPI images of the disk around HD 15115, dubbed the "blue needle". Previous studies with STIS, SPHERE, and ALMA have shown a brightness asymmetry and suggested that two distinct dust belts might orbit the star. Our analysis resolves the disk within one arcsecond from the star and computationally forward model the disk. The residual of the image might show the possibility of a second disk, while a brightness asymmetry is not that clear within the analyzed angular coverage.

19. Prerana Khatiwada, PhD Student, Computer & Information Sciences, University of Delaware

Title: A Pilot Study of Browsing Behaviors to Inform Future Misinformation Interventions

Abstract: Misinformation online makes it hard for us to trust and verify the news we find online which is a problem for users, the technology industry, and society at large. Thus, developing new tools and methods to mitigate this threat is critical. However, while solutions such as redirecting users to authoritative content may be useful they risk biasing people while also invading their digital privacy. To explore challenges around and perceptions of interventions, we developed a browser plugin that tracks users' browsing behaviors and news articles read online. We then conducted a multi-part pilot study with 34 participants who completed an online survey, two weeks of application logging with our plugin, and follow-up debrief interviews. Our results show that the number of articles reads and the News Media Literacy Score seem to be positively correlated and users perceive more value in the tools that help to combat misinformation and promote media literacy.

20. Greshma Vachepalli, MS Student, MS in Data Science Program, University of Delaware

Title: A GIS-enabled App for Mapping Salt-impacted Farmlands

Abstract: Saltwater intrusion (SWI) has become increasingly common in coastal regions due to sea level rise. SWI threatens coastal farmlands by creating conditions that are too wet and saline for crops to grow. This process leaves behind visual evidence of SWI on the surface of crop fields. We use drone, aerial, and satellite data to map the impact of SWI on farmlands in the Delmarva Peninsula from 2011-2013 and 2016-2017. Here we present a web-based mobile app that allows farmers and landscape managers to easily view changes to salt-impacted farmlands over space and time using interactive web maps. The app also provides the opportunity to improve SWI mapping efforts by giving the general public the ability to self-report locations where they observe salt patches.

21. Melanie Jimmerson, Undergraduate Student, Behavioral Health and Nutrition, Delaware State University

Title: Targeting TNFα protein signaling in Epithelial Intestinal cells to inhibit Inflammation

Abstract: This research focuses on TNFα protein signaling which is one way in which epithelial cells send signals to other cells, received through the STAT-3 receptor to inflame cellular membranes. This research will utilize computational chemistry and python to understand and curate a drug that can either defer the TNFα protein signaling or build a drug molecule to covalently bind to the STAT-3 receptor inhibiting inflammation in the small intestine. This silico-research approach to further understanding the mechanisms of Crohn's and autoimmune diseases will further diversify the discussion of food consumption's role in the progression or hindrance of chronic diseases. The further implications of this research include the nutrigenomics through the relationship between microbes in commonly consumed foods and Crohn's Disease and other chronic diseases.

22. Nina Rhames, Undergraduate Student, Chemistry & Biochemistry, Delaware State University

Title: Utilizing a Convolutional Neural Network for Drug Development of an ADAM17 Inhibitor

Abstract: Drug discovery is an expensive and time consuming process, especially in the era of new technology, such as personalized medicine where tremendous experiments and analysis are needed before bringing new drugs to the market. While In vivo and In vitro experiments are expensive, In silico methods become important and they can reduce the cost in drug discovery by prioritizing the experiments in more efficient ways. In this paper, we developed a convolutional neural network (CNN) to develop new small molecule inhibitors of ADAM17 – a protein involved in the pathogenesis of inflammatory bowel disease (IBD). The algorithm employed was a Junction Tree Autoencoder. This method developed over 50 novel compounds that were then tested via an ML algorithm previously developed. In the future, these molecules will be tested for their inhibitory potential.

23. Anjani Bhatia, PhD Student, Chemistry & Biochemistry, University of Delaware

Title: Predicting the Structure of the Intrinsically Disordered N-terminal Arm of Brome Mosaic Virus

Abstract: Brome mosaic virus (BMV) is a T=3 icosahedral RNA virus, 28 nm in diameter, that infects plants and causes stunting and mosaic symptoms. It has been used as a model to study gene expression, virus-host interactions, RNA replication, recombination, and encapsidation by positive-strand RNA viruses. The BMV Coat Protein (CP) has a globular domain flanked by an extended N-terminal arm (NTA) and a shorter C-terminal tail. The N-terminal 27 amino acids of the NTA are highly basic, required for RNA packaging. Post-translational modifications, such as phosphorylation of NTA influence the interaction of viral RNAs with the capsid. Because the NTA is intrinsically disordered, no structure has ever been determined. Here, we use all-atom modeling and molecular dynamics simulations to predict the structure of NTA in functional, RNA-binding conformations and investigate the role of phosphorylation in RNA packaging.

24. Salman Khan, Postdoctoral Researcher, Delaware Energy Institute, University of Delaware

Title: Characterizing supported metal cluster catalysts via actively trained machine learning potentials

Abstract: Catalysis is at the heart of chemical transformations. Supported sub-nanometer metal clusters are active for various industrially important reactions. However, unlike ordered catalysts, like metal/metal oxide crystals and zeolites, supported clusters have a distribution of active sites and they cannot be precisely characterized using spectroscopic methods. Furthermore, they present an intractably large configurational space, which cannot be reliably sampled using expensive ab initio computational methods. Consequently, the distribution of active site environments and structure-activity relations for these catalysts are poorly understood. In this work, we develop actively trained machine learning potentials (MLPs) for supported clusters. A global optimization method discovers stable clusters and an MLP is iteratively trained with the discovered clusters. We apply the framework to discover stable configurations of Al2O3 supported Platinum clusters (active for propane dehydrogenation).

25. **Suhotro Gorai, Master's Student, Center of Bioinformatics & Computational Biology , University of Delaware**

    Title: Visualizing the global lens epithelial cell injury response

    Abstract: Cataract is treated by surgical lens fiber cell removal followed by intraocular lens implantation. However, the lens epithelial cells (LECs) remaining behind post-surgery undergo injury response, reducing treatment effectiveness. Our lab has generated numerous RNA-seq datasets that reveal the time course of transcriptomic changes occurring in response to surgery. However, these large datasets are cumbersome to query simultaneously limiting their utility in hypothesis generation. Here we develop a user-friendly, interactive data visualization tool for the lens injury response time series (LIRTS). Existing RNA-seq datasets from wildtype mouse LECs at 0h, 6h, 24h, 48h, 72h and 120h post injury were reanalyzed using a standard pipeline incorporating edgeR. R Shiny package was deployed for data visualization. The LIRTS viewer allows users without bioinformatics experience to visualize the expression time course for any gene of interest via both a normalized boxplot and a scatterplot.

26. **Cameron Frank, PhD Student, Physics & Astronomy, University of Delaware**

    Title: Including the Effects of Magnetic Fields in Simulations of Inertial Confinement Fusion

    Abstract: In inertial confinement fusion (ICF), a high-powered laser rapidly compresses a spherical gas-filled shell for producing the high central temperatures in excess of 5 keV needed for high fusion yield. The interface of the shell and gas is susceptible to the Rayleigh-Taylor instability (RTI), which degrades the fusion yield by distorting the shell. These distortions seed self-generated magnetic fields, which can affect the implosion dynamics by modifying heat transport. The in-house code DEC2D simulates the RTI development during the stagnation-phase of ICF implosions. In this work, magnetohydrodynamics (MHD) solvers have been added into DEC2D. MHD solvers allow for the simulation of the effects of magnetic fields on fluid dynamics. We find that magnetic fields of about 250 MG are produced at bang time, with corresponding Hall parameters greater than 1. We find the Righi-Leduc transport causes a decrease in yield when MHD terms are included.

27. **Michael Wang, Staff, Center for Bioinformatics & Computational Biology, University of Delaware**

    Title: Sequence Embedding for UniRef Protein Clustering

    Abstract: In UniProt , we cluster 380 million proteins into clusters at three sequence similarity levels —UniRef100 (100%), UniRef90 (90%) and UniRef50 (50%) respectively. We are exploring a new pairwise similarity prediction method that takes advantage of protein sequence embedding. The idea is inspired by both SGT and ProtVec where the letter transition probabilities can represent unique features of sequences with long term dependency. We defined a vector space that potentially better address both factors by combining the advantages of both, adding up transition probabilities from AB to C to a limited distance with exponentially lowering weights. With length grouping, the sampled sequence embedding vectors' pairwise cosine value has shown a significant linear correlation (0.75-0.85) with sequence identity obtained through protein BLAST alignment (where the BLAST has hit). We plan to train AI prediction models with the embedding vectors and achieve fast clustering through the process.

28. **Yasmeen Olass, Undergraduate Student, Chemistry & Biochemistry, Delaware State University**

    Title: Using QSAR tofind medicinal compound from lemon grass to inhibit mosquito based cpA neuron receptors

    Abstract: In the tropical areas of Asia, the plants Cymbopogon citrates (Lemon Grass) and C. Nardus (Citronella Grass) have many medicinal components in the Native Asian culture that has not been proven in the scientific world. Cymbalom citrates contain citronella oil, a musk scent that attracts mosquitoes, such as carbon dioxide and Lactic acid found in humans. The citronella oil ingredients help block the scents sensed by mosquitoes, helping reduce the mosquitoes' landing by around 40%. This study will focus on developing a Quantitative structure- activity relationship (QSAR) model to predict what compounds found in these grasses can be used as an insect repellent from its essential oil obtained through steam distillation with the addition of using computational chemistry to inhibit the CpA receptors. CpA neurons are nerve cells that found within female mosquitoes, the CpA neurons are housed in capitate peg (cp) sensible on the maxillary palms and expresses the CO2 receptor.

29. **Janae Barnes, Undergraduate Student, Chemistry & Biochemistry, Delaware State University**

    Title: Utilizing Artificial Intelligence for the Optimization of Polymeric Materials for Drug Delivery

    Abstract: There are numerous polymers that can be used for drug delivery, but the effectiveness of each one varies. Two commonly used polymers for drug delivery include poly(glycolic acid) (PGA) and poly(lactic acid) (PLA). Since PGA is a polymer used for drug delivery, the next focus is how to create nanofibers for delivery. Many fabrication methods of PGA nanofibers exist, with no agreed upon optimization method. This study was conducted to utilize machine learning to create a database to find the best method of fabrication. Scientific peer-reviewed journals were used to create a database containing different fabrication methods and their results. This database was then used to create a machine learning model to predict the outcome of experimental parameters for PGA production. The concept can be evaluated and confirmed to be a potential solution in the future, however the application of PGA as well as other polymers may need to be further developed to translate successfully in the human body.

30. Santiago Antolinez, PhD Student, Chemistry & Biochemistry, University of Delaware

Title: Forcefield Interoperability: Implimenting AMBER forcefields into NAMD for Large Scale Simulations

Abstract: Molecular Dynamics (MD) is a widely used technique that can be used to study multimillion atom systems at the atomistic level. A key component of classical MD are forcefields, parameters which dictate the movement of biomolecules. Some of the most widely used forcefields are those corresponding to the AMBER family of forcefields (AMBERff). Currently, the native AMBER engine has poor scaling as system size increases . Furthermore, the interoperability of AMBERff with other MD engines is limited, making the use of AMBERff in large scale simulations unfeasible. Here we present an implementation of several forcefields in AMBERff to be read natively into NAMD, the leading MD simulation engine for multimillion atom systems. The results show the implementation to be accurate and stable, matching single point energies calculated in AMBER. In addition, our implementation is able to reproduce physical properties of several well-characterized biomolecules.

31. Tiara McKnight, Undergraduate Student, Chemistry & Biochemistry, Delaware State University

Title: Fabrication of Nanofiber Scaffold Matrices with the Use of Machine Learning

Abstract: Poly Lactic Acid (PLA) is a polymer that is not only very biocompatible but also biodegradable. It can be sourced organically from carbohydrates such as corn starch or sugar cane. Due to its ability to degrade into lactic acid, carbon dioxide, and water, it can safely be metabolized by the the body making it a perfect polymer to potentially use in medical applications. The fabrication methods of PLA nanofibers are far and wide, with no particularly agreed upon optimization method. This study, therefore, was conducted to utilize machine learning to find the best method of fabrication.This database was then used to create a machine learning model to predict the outcome of experimental parameters for PLA production. The concept can be evaluated and confirmed to be a potential solution in the future, however the application of PLA as well as other polymers may need to be further developed to translate successfully in the human body.

32. Poster withdrawn

33. Pragya Shrestha, PhD Student, School of Education, University of Delaware

Title: A Comparison of Three Effect Size Indices for Count-Based Outcomes in Single-Case Design Studies

Abstract: In Single-Case Designs(SCDs), three of the recently proposed effect size(ES) methods for count outcome data are: Nonlinear Bayesian(NLB), Log Response Ratio(LRR), and Bayesian Rate Ratio(BRR). The current research aims to investigate the performance of these ES methods using Markov Chain Monte Carlo simulation under various conditions of autocorrelation and overdispersion for a typical SCD. For this, 5000 datasets each were simulated for three subjects under the simulation conditions. To run the NLB and BRR models for each dataset in R, it takes approximately 80 seconds and 13 seconds respectively with 2-core processor. To reduce computational time, it is planned to utilize the processing capabilities of the Darwin HPC at the University of Delaware, which has the potential to cut computing time from 6,000 hours down to as little as a few hours (depending on number of cores and load).

34. Andres Holland, PhD Student, Hospitality & Sports Business Management, University of Delaware

Title: Food Delivery across Restaurant Classes: What text mining can teach us about customer experiences

Abstract: While numerous factors influence the decision to utilize online food delivery, the primary motive is the convenience and timesaving aspects the services provide. This research deviates from prior work by explicitly investigating customer delivery reviews to understand the customer experience. Specifically, our study scrapes publically available data posted on GrubHub from 188 restaurants located within 10 miles of Wilmington, DE. The sample comprises 8,850 reviews that were analyzed through a variety of text mining steps (data cleansing, stemming, stop word removal, vectorization). We are now implementing latent semantic analysis to identify topics that are associated between positive and negative reviews across restaurant categories (Quick-Service, Fast-Casual, Casual Dining). The results of the topic modeling should identify important delivery characteristics and attributes (speed, service, pricing, food quality, and packaging) that these unique segments should prioritize.

35. Muhammad Hani Zaheer, PhD Student, Physics & Astronomy, University of Delaware

Title: Quantum metrology algorithms for dark matter searches with clocks

Abstract: Quantum metrology aims to enhance the sensitivity of quantum sensors, such as atomic clocks, to signals while minimizing noise, using techniques from quantum information science. Atomic clocks have recently seen significant advancements in accuracy and are highly sensitive to changes in fundamental constants, making them ideal for searching for local ultralight scalar dark matter. The proposed nuclear clocks based on thorium 229m isomer are expected to offer even greater sensitivity. This study evaluates the use of various quantum metrology algorithms in dark matter searches using quantum clocks, proposing a new broadband algorithm and comparing it with previous protocols like zero dead time differential spectroscopy and narrowband dynamical decoupling. Numerical simulations are conducted to assess clock measurement protocol potential in detecting scalar dark matter, considering realistic sources of noise and dark matter decoherence.

36. Yahira Rivera, Undergraduate Student, Mathematical Sciences, Delaware State University

Title: FTIR and Raman Spectra of Concentrated Carbohydrate Solutions

Abstract: In this project, we measured FTIR and Raman spectra of three compounds -Ficoll, Alginate, and polyethylene glycol- dissolved in water at different concentrations. The measured raw spectra display complex sets of peaks, including those of fused silica and water. As the concentration of each compound increases, the intensity of the Raman peaks increases while the intensity of the water peaks decreases.

We combined the intensity correlation analysis (ICA) to locate the peaks and to assess changes of the peaks when the concentration is increased. We also used Principal Component Analysis to assess the effect of the concentration. ICA indicates an overall linear trend and closed loops likely due to changes of the peak profiles. PCA analysis shows systematic trends in PCA components. The results demonstrate how the combination of all tools can provide complementary insight for chemical analysis in crowded and concentrated samples

37. César Claros, PhD Student, Electrical & Computer Engineering

Title: Mechanical Property-Based Brain Age Prediction using Convolutional Neural Networks

Abstract: Brain age is a quantitative estimate to explain an individual's structural and functional brain measurements relative to the overall population. Brain age can be determined through neuroimaging techniques such as magnetic resonance imaging, computed tomography scans, or magnetic resonance elastography. Brain age predictions are valuable in describing differences related to developmental or neurodegenerative pathologies such as Alzheimer's or Parkinson's disease, which negatively impact brain mechanical integrity. We propose to quantify age-related brain changes processing brain's mechanical properties with a convolutional neural network to provide a single value estimate of an individual's brain age relative to a healthy chronologically aged cohort.

38. Abdul Rehman, PhD Student, Physics & Astronomy, University of Delaware

Title: A Deep learning approach to the Classification and De-noising of Cosmic-Ray Radio signals

Abstract: Cosmic rays (CRs) are high-energy particles of extraterrestrial origin. These CRs produce air showers upon entering Earth's atmosphere, emitting radio signals as charged particles in the air showers are deflected by Earth's magnetic field. Radio signals from air showers carry information about the energy and direction of the incident CRs. Interference, such as human-made radio noise and Galactic background, often complicates radio detection. This study presents a Convolutional Neural Network (CNN) method to classify and reduce background in radio signals. The CNNs were trained using Monte Carlo simulations of air shower radio signals and background data from an IceTop prototype station at the South Pole, using DARWIN's state-of-the-art GPUs for acceleration. Our results indicate that the use of CNNs significantly improves the accuracy of air shower radio pulse arrival times and amplitudes, which can lead to a more precise reconstruction of CR properties.

39. Parinaz Barakhshan, PhD Student, Electrical & Computer Engineering

Title: CaRV Tool, An Automated Tool for Capturing, Replaying and Validating Results of Experimental Sections in Science and Engineering Applications

Abstract: This poster presents an automated tool for capturing, replaying and validating (CaRV) results of experimental sections in science and engineering applications. An experimental section is a section of code that is to be tested or experimented upon. The tool instruments the application code provided by the user and gathers all the necessary information in order to run the experimental section without having to re-run the entire application. CaRV allows users to make changes to their long-running applications and measure the accuracy and efficiency of the changes without having to re-run the entire application. This automated tool enables users to quickly evaluate the efficacy and accuracy of changes made to scientific applications..

40. Dmytro Filin, PhD Student, Physics & Astronomy, University of Delaware

Title: Precise Atomic Structure Calculation with CI+All-Order Method on Highly Charged Nickel Ion Ni12+

Abstract: The highly charged ions (HCIs) such as Ni^{12+} are promising candidates for the next generation of atomic clocks; the spectra of HCIs are used for identifying the abundance of elements in astrophysical objects, and in addition, HCIs open intriguing opportunities for probing new physics beyond the standard model of particle physics. All of such prospective areas of HCI implementations require precise atomic structure calculations. In this work, we demonstrate obtaining accurate energy levels for the first four excited states of Ni^{12+} with help of precise CI+All-order technique based on the configuration interaction (CI) and linearized coupled cluster methods (CC). Especially, our efforts were focused on determining the energy of the second excited state of Ni^{12+} 3s^{2}3p^4 $^3P_0$. Experimental measurement of this energy is quite difficult and its value has the accuracy of $\pm$ 100 cm^{-1}. Such accuracy is very low for the possible clock transitions. Our calculations show that this uncertainty in the energy level can be significantly narrowed.

41. Zayna Juracka, Undergraduate Student, Engineering Physics, Delaware State University

Title: Physics-based adaptive learning to resolve overlapping molecular line transitions in mid-infrared spectroscopy

Abstract: Mid-Infrared laser-based sensing using molecular spectroscopy is commonly used for trace-gas detection and density measurements. An obvious advantage in detection in the mid-IR region is the fundamental absorption bands of several molecular species of interest for environmental, biomedical, and industrial processing applications. Several challenges in mid-IR sensing are due to significant interference and overlapping line transitions of molecular species with broad collision linewidths. Therefore, in many instances, the absorption signal is congested, overlapping line transitions of disparate molecular oscillator linestrenghts. In this project, we show a novel experimental methodology integrated with adaptive learning techniques to discriminate, quantify and resolve overlapping line transitions of nitrous oxide, water vapor, and carbon monoxide in the spectral region of 4 um to 10 um. The trace gas detection and machine learning-based classification method utilize the structural complexity of higher harmonic wavelength modulation spectroscopy signals that encode molecular collision dynamics information.

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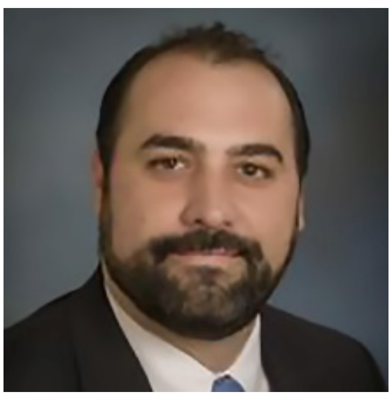

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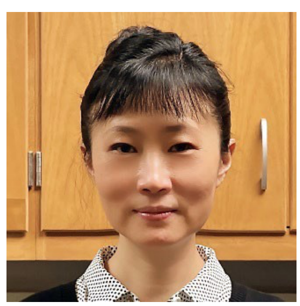
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