RapidPhage: a Microfluidic Based Phage Isolation Platform to Combat Antibiotic Resistant Pathogens

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In 2019 alone, antibiotic-resistant (AR) bacterial infections impacted over 3 million Americans, with a death toll of 48,000. By 2050, researchers predict that AR pathogens will globally cause over 300 million deaths, resulting in $100 trillion direct and indirect losses. To avoid such a catastrophe, researchers have increasingly explored antibiotic alternatives. Bacteriophage, aka phage, is a virus that specifically infects bacteria and has historically been used to treat bacterial infections before antibiotics. However, conventional methods to isolate such phages are slow, tedious, and inconsistent with modern drug discovery processes. We are developing a high-throughput microfluidic platform to rapidly isolate effective phages in a fraction of the time, named "RapidPhage". Thus far, we have established conventional methods for isolation of phages against Methicillin-Resistant Staphylococcus aureus (M.R.S.A.) from sewage samples. Irrespective of the sewage sample origin, conventional methods produced approximately 103 plaque-forming units against MRSA. Our developing RapidPhage platform will be used to compare against the phage titer efficacy of conventional methods. Since microfluidic co-capturing efficiency is very high, we expect that the RapidPhage platform will improve phage titer values by over 100-fold. Additionally, this developed platform should also recover more diverse MRSA-specific phages compared to established conventional methods. To exploit these viruses as therapeutic agents, we also plan to determine pharmacodynamics of the most robust phages, such as reproducibility factors and infection turnover rates. In conclusion, the developed RapidPhage will be a swift, robust, and highly efficient method for phage isolation to combat the rise of AR.

Residue Quality Affects Litter Decomposition Dynamics and Carbon and NitrogenMineralization in a Semi-arid Agroecosystem

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Although cover cropping is promoted to improve soil health in arid and semi-arid environments, information on its residue decomposition and soil carbon (C) and nitrogen (N) dynamics is very limited. This study aimed to evaluate decomposition dynamics and nutrient release from different winter cover crops in a semi-arid agroecosystem. Twenty grams of triticale (Triticale hexaploid Lart), turnip (*Brassica rapa* subsp. *rapa L),* and pea (*Pisum sativum* subsp. *arvense L*) cover crops residues were kept in litter bags and deployed in the field. After cover crop termination forage sorghum (Sorghum bicolor L) was planted as a subsequent cash crop. The treatments were arranged in a randomized complete block design (RCBD) with four replications. Litter bags were removed every other week (a total of 12 destructive samplings) to evaluate the remaining dry matter and C and N contents. Also, a 10-week long incubation was set in laboratory conditions to understand the decomposition of triticale, turnip, pea, wheat, sorghum, and native grass residues by estimating potential mineralizable carbon (PMC) each week. After 98 days, the residue decomposition in litter bags was higher with pea (47 %) followed by turnip and triticale (both decomposed 40 %). The residue analysis showed that legumes lower C: N ratio favored faster decomposition. Residue types and quality both affected the decomposition rates. Cover crop termination and cash crop planting times should be managed based on the quality of crop or cover crop residue for effective soil nutrient cycling and their uptake by subsequent crops.

Analysis of Asynchronous Communications on Microgrid State Estimation

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Average consensus algorithms in microgrids are becoming attractive concepts to meet the increasing demands for energy. The goal of the average consensus is to calculate the average of initial values across dispersed nodes by sharing data via communications. The Average Consensus Theorem relies on the local information of agents to guarantee that important information is shared in a distributed way. It is known that synchronization is necessary to obtain an accurate average across the distributed nodes. Due to several technical issues, however, such as the requirement of a global clock and random packet drops/delays, which may occur during the implementation stage, the synchronous model is highly limited in reality. An asynchronous model, a synchronous one's counterpart, naturally takes into consideration the problems mentioned above and is thus more practical. The only downside of the asynchronous model is that it may result in inaccuracies in the consensus value which requires more thorough investigations. To this end, the performance of different network topologies has been investigated in this study for asynchronous systems with 16 different agents and random initial values. We analyzed three important performance factors: the convergence speed, error bound width with respect to the exact value, and the error variance.

NMHU-BioPACIFIC MIP PREM Website

Justice Ainsworth, New Mexico Highlands University

There are different ways to build a website, which require the knowledge of multiple programming languages. To structure a website the most common languages used are HTML, JavaScript, Python, SQL, and PHP. The most common languages used for styling the website are CSS and Bootstrap. To determine which language was best for this website each programming language was researched and the four languages that were chosen were HTML, JavaScript, CSS, and Bootstrap 5. These languages allow for a smooth process for building the NMHU-BioPACIFIC MIP PREM website.

Examining Spatial Heterogeneity and Tourism Potential of Water Resources in New Mexico

Jason Banegas, New Mexico State University

Increasing outdoor tourism in New Mexico and the growing demand for water-based tourism amenities requires developing innovative strategies for resource allocation and service integration among many existing and potential recreation locations. Identifying tourism potential and optimizing resource allocation has been addressed in studies using a multitude of models, methods, and algorithms; however, variations between the influential factors of tourism locations are best analyzed with a Geographical Information System (GIS) based research model that can examine diverse spatial relationships in these environments. This study uses a Geographically Weighted Regression (GWR) method to illustrate that variables related to drivers of tourism are locally distinct. This tool is used to examine the spatial non-stationarity of relevant water-based tourism variables. Spatial discrepancies are shown to exist in the explanatory variables useful for developing tourism resources in rural and urban locations in the New Mexico study area. This GWR analysis can strengthen the decision process and allow policymakers to identify distinct influential factors and areas where resources for expanding water-based tourism should be focused.

Wall-Modeled Large Eddy Simulations of Turbulent Boundary Layer over a Flat-Plate for Aero-Optical Distortion Analysis

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Density fluctuations due to compressible turbulent boundary layers cause significant aero-optical distortions that deteriorate the performance of sensors and directed energy applications. As part of a multi-institutional research team led by Sandia National Laboratories, compressible wall-modeled large-eddy simulations of turbulent flat plate boundary layer flows were carried out for Mach 3.5, 7.87, and 13.64. The Mach 3.5 conditions are the same as for a reference direct numerical simulation (Miller et al., 2021). For the Mach 7.87 case, the Sandia Hypersonic Wind Tunnel freestream values were matched. The Mach 13.64 case was modeled after the freestream conditions inside the Arnold Engineering Development Complex Hypervelocity Tunnel 9. Despite the relatively low grid resolution compared to reference direct numerical simulations, the mean velocity, temperature, and Reynolds-stress profiles obtained from the wall-modeled simulations are in good agreement with available reference data. In addition, the normalized root-mean-square optical path difference obtained from the present simulations compares well with reference simulations and experiments. This suggests that wall-modeled large-eddy simulations can provide accurate and efficient predictions of the aero-optical path distortions at a drastically lower computational cost than direct numerical simulations. A semi-analytical relationship by Notre Dame University that was developed for low-Mach applications underpredicts the path difference for the higher Mach numbers. This mismatch provided the motivation for evaluating the underlying assumptions of the theoretical model for hypersonic boundary layer flows. The present results contribute to the development of updated models for the path difference that will assist the design of high-speed aero-optical applications.

Poster #14

Michael Holzmann, CCB, University of New Mexico
Pavel Yamanushkin, CCB, University of New Mexico
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Cycloalkynes and their utilization in cycloaddition reactions enable modular strategies spanning the molecular sciences. Strain-imparted by deviation from linearity-enables sufficient alkyne reactivity without the need for a catalyst (e.g., copper); though the design and synthesis of stable reagents with suitable reactivity remains an ongoing challenge. We report the incorporation of an endocyclic sulfate within a dibenzocyclononyne scaffold to generate a cyclononyne displaying remarkable reactivity and stability. Through computational analyses, we revealed that the endocyclic sulfate group shares nearly half of the total strain energy, providing an activation strategy that reduces alkyne bending. Rehybridization of alkyne carbons in the formation of the heterocyclic product relieves strain both at the reactive site and in the transannular sulfate group. This mode of remote activation enables rapid reactivity while minimizing distortion and strain at the reactive site (the alkyne). The result: a design strategy for a new class of cycloalkynes with increased stability and reactivity.

Late-Stage SuFEx Diversification of HIV Protease Inhibitor

Bipin Khanal, University of New Mexico

Click chemistry- a nature-inspired approach for rapid synthesis of useful compounds , since its dawn has dominated organic synthesis. Modern development of near-perfect reactions enables modular manipulation of building blocks. Our group has recently reported a mild route to SuFExable pyrazoles. We are now poised to rapidly explore unknown chemical space via controllable diversification of these densely functionalized heterocycles. Recent progress in late-stage modification of FDA-approved pharmaceuticals, especially for the treatment of HIV/AIDS, to unlock new properties will be presented.

A Deep Spatial-Temporal-Channel Attention Network for sEMG-based Hand Gesture Recognition

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Zhirui Luo, New Mexico Institute of Mining and Technology
Ruobin Qi, New Mexico Institute of Mining and Technology
Zheng Jun, New Mexico Institute of Mining and Technology

Hand gesture recognition has become more attractive in the field of human-computer interaction (HCI) due to the rich information and the natural and intuitive communication mode provided by hand gestures in human dialog. Many computer vision-based approaches have been applied to hand gesture recognition but the strict requirements of background invariance and lighting insensitivity limit their accuracy and robustness. Compared with vision-based approaches, methods using surface electromyography (sEMG) signals are more robust and have better usability. In this work, we proposed a new deep learning model for hand gesture recognition using multi-channel sEMG signals, which consists of a ResNet50 network and a novel triple attention module. The ResNet50 network serves as an implicit automated feature extractor to retrieve features from the sEMG signals. The triple attention module combines spatial attention, temporal attention, and channel attention to signify important features for hand gesture recognition. The performance of the proposed model is evaluated with two popular datasets, Ninapro-DB1 and Ninapro-DB2. The results demonstrate that the proposed model significantly outperforms the existing state-of-the-art methods.

A Deep Attention Network for Non-intrusive Building Occupancy Detection Using Smart Meters

Zhirui Luo, Computer Science, New Mexico Institute of mining and technology
Ruobin Qi, Computer Science, New Mexico Institute of mining and technology
Qingqing Li, Computer Science, New Mexico Institute of mining and technology
Jun Zheng, Computer Science, New Mexico Institute of mining and technology
Sihua Shao, Electrical Engineering, New Mexico Institute of mining and technology

Occupancy information is gaining more attention for efficient energy management in the building sector because it provides significant potential for energy reduction. The massive smart meter data collected by the advanced metering infrastructure (AMI) facilitates inferring occupancy status in a non-intrusive way, but the non-linear relationship between power consumption data and building occupancy status hampers the effectiveness of detection techniques. Current machine learning as well as deep learning models are restricted in manual feature extraction and hard to scale up when facing massive smart meter data. In this work, we propose a deep attention network called ABODE-Net which utilizes a novel parallel attention block to infer real-time building occupancy status from raw smart meter data and corresponding time information in an end-to-end manner. We compared our method with a set of state-of-the-art shallow machine learning and deep learning models using two smart meter datasets widely used for building occupancy detection. The results show that ABODE-Net has a significantly better performance in all experimental cases. This study proves the validity of the proposed ABODE-Net as a solution for non-intrusive building occupancy detection using smart meter data.

Hydrogels as Support Medium for the Culture of Cyanobacteria

Brannette Mejia, Los Alamos National Laboratory

Cyanobacteria are prokaryotic cells that have the ability to perform photosynthesis. Spirulina (*Arthrospira Platensis*) is a common cyanobacterium that can be a food source for animals and humans, as well as possess characteristics such as biosorption and bioaccumulation capacity. Hydrogels are hydrophilic polymers that do not dissolve in water, instead, they tend to absorb water, by possessing hydrophilic functional groups. They can be formed by utilizing natural polymers and adding crosslinkers when together creating a solution with high viscosity and consistency. Hydrogels have a vast variety of applications, mostly in the biomedical field such as contact lens production, wound dressings, 3D printing, and agarose. In this project, we study the use of poly(vinyl) alcohol as a polymer matrix in combination with borax as a compatible crosslinker. In this work, we first explore various parameters to produce self-standing hydrogels that can be cast, or 3D printed into various shapes. We also investigate the viability of Arthrospira Platensis in a hydrogel medium. A wide variety of techniques are employed to determine the microscopic features as well as the mechanical and chemical properties of the hydrogels.We show that after forming 6 different hydrogels with a variety of concentrations, the level of PVA and borax that is added to the solution has a direct effect on the hydrogel behavior. Our results identified that the 5% PVA and 4% Borax hydrogel showed the utmost characteristics and properties that matched the expectations of hydrogel behavior. LA-UR-22-30293

Isoreticular Synthesis of HKUST-Type Metal-Organic Framework Using Imine Functionality

Dr. Tatiana Timofeeva, Department of Chemistry, New Mexico Highlands University
Dr. Alisha Gogia

Metal-organic frameworks (MOFs), which is a class of hybrid organic and inorganic porous materials with 2D and 3D networks, have emerged as important materials which can be used for different purposes such as gas separation and storage, in the pharmaceutical industry as drug delivery compounds, and in environmental applications such as photoluminescent sensors. One of the main advantages which MOFs offers is the easy tunability of functionality in the resultant MOF structures by slight changes in the organic ligand. By choosing the right geometry of ligands and metal nodes it is possible to construct the target MOFs with high porosity and pore volume. One highly advantageous functionality which can be incorporated into the MOF assembly is the imine group. The imine group tends to have extensive H-bonding interactions with the guest/analyte molecules. This allows the sensing and sorption of various important molecules using MOFs. In addition, the imine functional group provides the advantage of post-synthetic modification to convert imine into amine for different applications such as water and gas separation, drug delivery, and luminescent sensing. In the current work, we have designed and synthesized an imine-based tricarboxylic ligand, 4,4,Äô,4,Äô,Äô-(((1E,1,ÄôE,1,Äô,ÄôE)-benzene))tris(azaneylylidene))tribenzoicasid (H3bttta), to incorporate in the HKUST-type MOF assembly using Cu(II) metal center as the node. HKUST was chosen as the target structure and isoreticular synthesis was done using the synthesized H3bttta for it offers large hexagonal pores which can encapsulate a bunch of analyte molecules. Furthermore, in addition to the functional benefits, we have also focused on the structural variations brought in by the flexibility of the H3bttta ligand to the resultant MOF structure. The study showcases the standardizations involved in the synthesis of the organic ligand and the MOF, and the characterization of the bulk powders.

Synthesis of Carbonyl-Functionalized p-Phenylenes for Probing Electron Delocalization

Chimezie Onukwuli, Eastern New Mexico University
Juchao Yan, Eastern New Mexico University

Organic pi-conjugated p-phenylenes have attracted enormous current interest, owing to their optoelectronic applications including organic solar cells (OSCs), light-emitting diodes, and organic lasers. The design of OSCs with an improved power conversion efficiency demands a proper understanding of electron delocalization and its influence on the energetics and dynamics of electrons. In literature, nitrile-functionalized ladder-type oligo (p-phenylenes) have been synthesized and used to probe electron delocalization by time-resolved infrared spectroscopy coupled with pulse radiolysis. While these rigid coplanar compounds are infrared-responsive and thermally stable, nitrile groups are not commonly incorporated into solar-related molecules. Herein, we propose the incorporation of a carbonyl group infrared reporter into ladder-type oligo (p-phenylene) architecture to further probe electron delocalization. The proposed compounds are being synthesized via palladium reductive carbonylation using N-formyl saccharin as a source of carbonyl. The target compounds are affordable and easy to manufacture, which is critical for the commercial production of donor materials for OSCs. In this poster, we focus on our molecular design, syntheses, and characterizations.

Novel Manganese-Halide 1-D and 2-D Frameworks and their Emission Properties

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RayVen Gonzales, New Mexico Highlands University
Dr. Tatiana Timofeeva, Department of Chemistry, New Mexico Highlands University
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In the past years metal-halide perovskites (MHPs) attracted much attention as they are exceptional candidates for novel photovoltaic materials. MHPs are not limited to photovoltaics and our goal at NMHU is to study manganese-halide perovskites (MnHPs) for their potential magnetic, ferroelectric, and light emission properties. These properties imply that these compounds can be used for LEDs and detectors. Manganese-halide compounds normally crystallize with isolated tetrahedral MnX4 units, however, they can crystallize in 1-D chains, or 2-D layers when organic ligands are present. Our group synthesized five new MnHPs, four of them with 1-D chains, and one of them with 2-D layers with 3-aminopyridine as the organic ligand. Our results show these MHPs can be modified by the amount of water present, and by the solvent used, leading to 1-D chains with different angles between manganese octahedrons.

Characterization of a Modified Carbon Fixation echanism in Synechocystis sp PCC 6803

Sara Pacheco, Los Alamos National Laboratory

Cyanobacteria are a promising platform for the production of carbon-neutral biofuels, plastics, and other commodities. However, these cyanobacterial-based technologies must improve in biomass yield and biochemical composition to compete with the economics of petroleum-based products. We seek to increase biomass production by improving the CO2 fixation capacity within the cyanobacterial cell. Towards this goal, we introduced a copy of the ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) type IC from the soil bacterium Cupriavidus necator H16 into the cyanobacterium Synechocystis sp. PCC 6803, which naturally expresses Rubisco-type IB within a carboxysome. We hypothesize that differences in Rubisco, IC cellular location, catalytic turnover, and substrate specificity in the transgenic PCC 6803 strains will complement its native CO2 concentrating mechanism, resulting in improved photosynthetic efficiency and biomass accumulation. We will test this through growth (spectrophotometrically at 730 nm), photosystem II fluorescence, oxygen evolution, and flow cytometry (dye-assisted evaluation of polyhydroxybutyrate accumulation) in cultures under various CO2 concentrations. Our success will improve the carbon fixation capacity of the cell, increase biomass production, and increase cyanobacteria,Äôs economic value.

Deep Feature Extraction for Semi-supervised Electricity Theft Detection in AMI with Observer Meters

Ruobin Qi, New Mexico Institute of Mining and Technology
Qingqing Li, New Mexico Institute of Mining and Technology
Zhirui Luo, New Mexico Institute of Mining and Technology
Jun Zheng, New Mexico Institute of Mining and Technology

Electricity thieves can launch cyberattacks against advanced metering infrastructure (AMI) to reduce their electricity bills which damage the integrity of the smart grid and causes huge economic losses to utilities. Traditional supervised learning-based methods rely on representative fraudulent data to train good detection models. However, it's hard to collect representative electricity theft data in the real world and a trained supervised model may not be able to identify new false data injection attacks. On the other hand, semi-supervised learning only employs normal data to train detection models which makes it suitable for detecting unknown attacks. To this end, we propose a semi-supervised deep learning method for electricity theft detection in AMI. The method uses ratio profile data calculated from observer meter data as the input. Deep features are extracted from the ratio profile data using continuous wavelet transform (CWT), deep representation learning, and principal component analysis (PCA). The extracted features are then fed into an autoencoder network for semi-supervised anomaly detection. The performance of the proposed method is evaluated with real-world smart meter datasets to demonstrate its validity for electricity theft detection.

Examining the Rights-of-Way for Navajo Allotment Lands in Connection to the Navajo-Gallup Water Supply Project

Bernadette Fontenelle, University of New Mexico

This research examines the Right-of-Way (ROW) process for the Navajo Nation, USA, allotment lands. Today, there are 573 Indian nations. Each Indian nation has its own history relating to Indian allotment lands. During the 1880s, allotment lands were created through a federal Indian policy. The policy approved various Indian reservation lands into allotment lands. Today, these allotment lands have become a ROW issue. This research examines a real example of the ROW issues impacting the Navajo-Gallup Water Supply Project (Project). Land access for allotment lands is questionable. Water access for the Project was secured and supplied through the Navajo Nation San Juan River Water Rights Settlement. The Project pipeline alignment will cross six types of land. Each type of land has its own ROW process. Several methods were applied to determine the ROW process for the Navajo allotment lands. A literature review of existing federal Indian policy finds that the Navajo Nation does not have authority over the allotment lands. Two federal sister agencies, the U.S. Bureau of Indian Affairs and the Bureau of Reclamation are challenged by the administrative ROW process. One has authority over these allotment lands, the other must initiate the ROW application of the Project. The Bureau of Indian Affairs will approve or disapprove of the ROW easement. After examination, the research identifies areas of improvement for the current ROW process and provides recommendations, starting with a better framework to implement into the ROW process for Navajo allotment lands. Water is Life!

iCAD: information-Centric network Architecture for DDoS Protection in the Smart Grid

George Torres, New Mexico State University
Sharad Shrestha, New Mexico State University

With the proliferation of differently-abled and heterogeneous devices in the smart grid, Denial of Service (DoS) is becoming an even more potent attack vector than before. This poster demonstrates the ease with which an adversary can orchestrate DoS and distributed DoS (DDoS) attacks on the grid. We propose iCAD, an information-centric architecture that extends the iCAAP architecture we previously proposed, complete with mitigation strategies built for DoS/DDoS resilience. We present our architecture and demonstrate the architecture and the mitigation technique's effectiveness in mitigating DoS/DDoS attacks in the face of significant attack load from the distributed agents.

High-Throughput Synthesis and Modification of Peptides

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Mark Aldren M. Feliciano
Pavel Yamanushkin

Expanding chemical space beyond the genetically encoded amino acids endows biomolecules with unique properties. As nature harnesses chemical (post-translational) modifications, we seek to incorporate synthetic modifications into peptide scaffolds. We are currently utilizing high-throughput techniques (i.e., phage display) to fabricate modified peptides to understand the role of peptide structure on employed techniques and synthesize biomaterials with utility in various applications.