UC-National Laboratory Fees Research Program
Abstracts for Active Awards

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Functional multimaterial hydrogels via dual-wavelength projection microstereolithography

Host Campus: Santa Barbara
Lead Investigator: Isabel Arias Ponce
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

Biological systems often incorporate hierarchically ordered structures of soft and hard domains that give tissues toughness and strain hardening response. While novel resins for light-based additive manufacturing (AM) have been extensively researched, the ability to pattern multimaterial objects remains a challenge. The goal of this project is to 3D print multimaterial, functional hydrogels which are critical to engineering biomimetic structures with regions of varying compliance and functionality. An example of this is the osteochondral interface, where stiffness gradients and robust interfaces between harder and softer domains are vital for load transfer with minimal damage over a lifetime of cycles. The main deliverables for this research are (1) to design a resin for dual wavelength, multimaterial 3D printing of hierarchical hydrogel structures and (2) to selectively pattern bioactive cues through active ester chemistry and peptide functionalization. This work will be enabled by combining the additive manufacturing (AM) systems and resin formulation expertise in Dr. Maxim Shusteff's group at LLNL with the polymer chemistry and photopolymerization expertise in the laboratories of Dr. Rachel Segalman and Dr. Craig Hawker at UC Santa Barbara. The Hawker lab has developed orthogonal photopolymerization resins to pattern multimaterial objects with chemically distinct domains and strong interconnected interfaces. The Segalman lab has developed a synthetic platform to fabricate functional hydrogel networks that can be substituted with libraries of ligands to selectively tailor the network's chemical functionality. The advanced manufacturing group at LLNL led by Maxim Shusteff has a cutting-edge, modular projection microstereolithography (PµSL) platform which has been adapted for dual wavelength patterning. By merging the core expertise at both institutions, this project seeks to 3DP dual wavelength, multimaterial hydrogels with versatile chemical functionality, varying mechanical properties, and high resolution control, to be demonstrated through a bioinspired osteochondral model. Success in this project will open the door to investigations of hierarchical multimaterial models for geometrically complex, bioengineered tissues and elucidate structure-property relationships towards the design of mechanically enhanced 3DP materials.

Laser-Based X-ray Radiographic Imaging for High Energy Density Science and Applications

Host Campus: San Diego
Lead Investigator: Alemayehu Bogale
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

X-ray radiography is an essential imaging tool across many fields. In high-energy-density plasmas, x-ray backlighting aids in extracting various physical properties from the system. The use of high-intensity lasers focused on high-Z foil targets produce relativistic electrons that generate MeV photons via Bremsstrahlung, Compton scattering, and synchrotron emission. The advantages over existing sources include smaller spot size, shorter pulse duration, tailorable spectra, and flexible configurations. This enables imaging with higher spatial and temporal resolution and multiple fields of view. The ability to resolve finer features on dense objects and capture physical processes on the order of picoseconds would be transformational; however, certain limiting factors must be addressed to achieve such a source.

Ideally, laser energy would be coupled to the front surface of the target and converted to x-rays at the rear surface. Typical short pulse lasers have pedestals prior to the peak pulse that create pre-plasmas near the front surface, reflecting a large fraction of incident energy. The x-ray dose increases as energy deposition is improved, and to that end the use of high-contrast lasers will minimize the pedestal that creates the pre-plasma. In addition, developments in target fabrication have permitted nano-structured and foam targets to be deployed. These system conditions introduce the relativistically induced transparency regime where the laser penetrates deeper into the target, yielding greater conversion efficiency.

While increases in efficiency are necessary, there must be stability in the spectrum and dose for the source to be a viable diagnostic. The object must experience uniform irradiation with minimal spot motion. Resulting pre-plasmas filament beams which in turn degrade the reproducibility of emissions. Experiments will quantify this stability and validate models that facilitate the design of radiographic systems for targeted applications. Addressing these factors will be possible using LANL's extensive resources, such as VPIC and MNCP transport codes that model the generation of hot-electrons and x-rays, respectively, and the lab's expertise in target fabrication and connection with high-contrast laser facilities. Ultimately, laser-based x-ray sources will enable new applications in the weapons program and broader scientific community.

Strengthening global food security by tracing pesticide mixture effects on honey bee health

Host Campus: Davis
Lead Investigator: Angela Encerrado
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

Honey bees are essential to global agriculture and food security. In the U.S., bees pollinate over 100 commercially grown crops and increase their values by over $15 billion each year, including the world's biggest pollination event of CA almond trees. Bee populations are in decline, with chronic colony losses driven by biological (parasites, pathogens), dietary (poor nutrition), climate (warmer, dryer) and man-made (pesticides) stressors. Risk assessments often focus on single pesticide safety profiles based on worker bee lethality tests. Yet, the effects of co-exposure to two or more pesticides and their metabolites have been poorly studied. In addition, low-dose effects of those compounds on the most essential members of a bee hive, the queen bee and her developing larvae, have not been evaluated.

To better understand how environmental mixtures of crop pesticides can enter, disperse, and accumulate within a beehive and promote synergistic toxicity to vulnerable colony members, I propose to trace and quantify radioactively labeled single and binary combinations of pesticides through biologically relevant matrices, from nectar to nurse bee to queen bee to larvae. The fate and levels of compounds will also be analyzed in bee products of human consumption and commercial interest, honey and wax. Such studies are often hampered by the small amounts of chemicals and metabolites that are exchanged via food (trophallaxis) between hive members and the inability to trace a pesticide metabolite detected in bee products back to its biological source within the hive. These sensitivity challenges lead me to the unique Biological Accelerator Mass Spectrometry (AMS) facility at LLNL to trace non-lethal amounts of radiolabeled pesticides. Dr. Bruce Buchholz is an expert in biological tracers and has successfully applied AMS to study pesticide levels in Argentinian ant colonies.

This project aims to characterize the biochemical flow of pesticides through a bee colony and to locate and mitigate biological sinks within the hive. The immediate goal is to help beekeepers to develop replacement strategies to assure survival of a colony. The long-term goal is to systematically analyze multiple pesticide exposures to inform regulatory guidelines on best bee and pesticide management strategies to improve the economic value of pollination and food security in the U.S.

Tunable 2D conducting oxide epsilon-near-zero and metasurfaces for high power laser applications

Host Campus: Irvine
Lead Investigator: Christopher Gonzalez
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

The optical response of epsilon-near-zero (ENZ) metasurface/material has gained significant interest recently as these materials show near-zero permittivity and exhibit unique optical properties, including strong optical confinement and abnormal light-matter interaction and optical nonlinearity. While ultrathin ENZ metasurfaces are promising for the ultrathin and lightweight photonic components and devices, several fundamental challenges limit the use of current ENZ optical materials for practical optical applications, including (1) low power operation because of high optical losses (2) limits to the maximum achievable optical confinement in conventional bulk ENZ materials (3) lack of efficient tunability due to the fixed electron density of the metallic or semiconducting ENZ material.

This proposal opens a new scientific direction for tunable ENZ metasurfaces by developing novel 2D ENZ materials with low optical losses, high damage threshold, and large tunability, overcoming the limitations of conventional materials and opening the field of nanophotonics and metamaterials of 2D materials for novel optical and laser applications that require exceptionally fast speeds and exceptional precision. We will develop tunable 2D ENZ metasurfaces for high power laser applications and perform this project using the high-power laser characterization facility at LLNL and the ENZ material fabrication and characterization in Lee's Lab at UCI. This project is significant because it will enable implementation of novel electrically tunable 2D ENZ devices, such as beam steering devices and optical switches/limiters, with high operation speeds, low energy consumption, and high power operation for advanced high power laser technologies for defense, imaging/sensing, and telecommunication. This fellowship program also exploits LLNL's Lasers and Optical Science and Technology core competency. It is relevant to the use of advanced optical metasurfaces in the Directed energy focus area, enabling better performance of steering and aberration correction of laser beams. It is also strongly aligned with LLNL's core competency in Advanced Materials and Manufacturing for laser-based systems for additive manufacturing using 3D volumetric printing and selective laser melting of powder beds, enabling better accuracy and speed of the raster beam system and thus scalability.

Molecular Simulation to Enable Novel Target Generalization of Structure-Based Deep Learning Models

Host Campus: San Diego
Lead Investigator: William Jones
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

Recently, the DOE has funded efforts involving multiple national laboratories to develop therapeutic treatments for emerging biothreats, namely SARS-CoV-2 (National Virtual Biotechnology Laboratory or NVBL). The known drug-like chemical space is regularly cited as being on the order of 1e60 possibilities and experiment feedback can occur on the order of days or longer. Atomistic Molecular Dynamics (MD) simulations have made progress as comparatively rapid computational feedback mechanisms that produce atomistic descriptions of biomolecules over a temporal scale that serve as the basis for SOA methods for ranking potential lead molecules predicted to interact with a target protein. It is well documented that MD simulations require specialized computing architectures to reach relevant timescales. MD simulations also exhibit poor sampling efficiency in exploration of configuration space, which is a primary focus of current MD research.

Structure-based deep learning methods (SDL) trained on experimentally derived atomistic “snapshots” have demonstrated the ability to perform competitively to more expensive MD-based scoring methods. SOA-competitive SDL methods developed and applied at LLNL on several projects to rank potential SARS-CoV-2 viral protein inhibitors have highlighted significant challenges. SDL methods lack dynamic information of the interaction and are subject to limited experimental training data. MD has seldom been explored in the literature to address these issues.

A better understanding of the tradeoffs between combinations of various SDL architectures and data collected from representative MD simulation algorithms would provide a significant improvement in the current understanding of approaches to incorporate dynamics information to improve SDL generalization to novel protein targets. We then propose to develop an improved model based on our insights and current approaches in the literature to then retroactively compare with previous approaches developed and applied at LLNL. The combination of prior SDL research and current relationships with simulation experts at LLNL put our team in a unique position to leverage LLNL GPU clusters such as Lassen, access to high-quality molecular simulation engines such as Amber, extensive prior experience with deep learning frameworks such as PyTorch, and existing data generated from prior related projects.

Supernova Shockwaves: Searching for Observational Clues on How Stars Die

Host Campus: Berkeley
Lead Investigator: David Khatami
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

Astrophysical observations of stellar explosions contain a wealth of information on the nuclear processes occurring in the evolution and eventual death of massive stars. In recent years, astronomers have discovered that many stars shed off their outer layers near the end of their lives. Once the star dies, the supernova explosion slams into the expelled material, creating a highly energetic shockwave that is observable across the entire electromagnetic spectrum. However, the resulting emission remains poorly understood, as it involves the complex interplay of atomic-scale physical processes manifesting in a cosmic-sized shockwave. Previous attempts to simulate the shockwave emission have used overly simplified models in order to be computationally feasible; as such, these models have been limited in their predictive power.

As it turns out, supernova shockwaves bear a great deal of resemblance to structures that appear in the context of fusion and high energy density science. Many of the diagnostic tools used in modeling fusion experiments, such as the CRETIN code at Lawrence Livermore (Scott & Hansen 2010), are identical to those used in our astrophysical context. However, the capabilities of such codes are more mature and extensive than those in use by astrophysicists to model stellar explosions; the computational advancements in fusion codes have yet to make their way into astrophysics. As such, supernova codes are not able to fully utilize the capabilities of current supercomputers.

We therefore intend to adapt these recent algorithmic and computational developments in fusion diagnostic codes to further our modeling capabilities of supernova shockwaves. These improvements, combined with advances in supercomputing capabilities, will enable us to realistically simulate supernova shockwaves to a degree that was previously unfeasible. Our simulations will supply astronomers with synthetic observables that can be directly compared to supernova shockwaves seen in the universe. Finally, these simulations will demonstrate how astrophysical shockwaves can help inform the field of high energy density physics more broadly, and provide context for the design of fusion experiments.

Tissue engineering of a biological periosteum using granular microgels

Host Campus: Davis
Lead Investigator: Sabrina Mierswa
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2026 *Amount*: $ 206,496

Abstract:

Despite considerable advances in bone repair, many clinical problems such as bone loss, defects, soft tissue damage, lack of ample mechanical stability, and infection play a crucial role in successful bone healing and must be addressed. The periosteum responds to physical insult and serves as a source of reparative cells at the injury site. Without the periosteum present, the bone's source of chondrogenic and osteogenic cells are absent when an injury to bone occurs. Current clinical approaches for regenerating the periosteum utilize autologous periosteum transplantation, but this strategy is limited by the tissue availability, morbidity, and increased risk of infection. Thus, there is a critical need to develop effective replacements for damaged periosteum.

Biomaterials provide an opportunity to create a tissue engineered periosteum (TEP) and replace its function. Compared to other approaches, granular microgels have distinct advantages over bulk materials that boast tunable parameters ranging from stiffness to porosity and can be used to easily generate gradients of relevant biophysical properties. Microgels are customizable building blocks that can be assembled to fabricate multi-material, multi-stiffness, multi-cellular scaffolds with tunable pore size. Polyethylene glycol (PEG) microgels are an ideal platform for a periosteum mimic due to their homogeneity in size and tunable properties in annealed form.

For this project, LLNL's biological laboratory facilities, Micro-fabrication facility, and bioprinting laboratory will be used. Further equipment and facilities used include mechanical characterization (e.g., rheometer, Instron, Chiaro nanoindenter) and the Buchi Encapsulator B-390. The nanoindenter and encapsulator are of particular interest to this project and are not found on the UC Davis campus. The knowledge and expertise of Dr. Moya and her team are also vital for the successful completion of this project. Animal studies will be conducted at UC Davis at the Sacramento medical campus to leverage the experience of orthopedic surgeons and expertise in treating bone defects in preclinical models. My previous work at LLNL, research experience, and technical training make me the ideal candidate for carrying out this work at LLNL. My career goal of holding a PI position at a national laboratory is also ideally situated for completing this work at LLNL.

Ultra High Temperature Material Synthesis and Degradation Mechanisms in Hypersonic Flight

Host Campus: Davis
Lead Investigator: William Rosenberg
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2023 *End Date*: 3/31/2025 *Amount*: $ 139,536

Abstract:

When traveling at hypersonic speeds in Earth's atmosphere, materials are required to operate under extreme conditions. The leading edge of a hypersonic vehicle must withstand temperatures up to 2727 ˚C at Mach 8, in addition to reactive oxygen environments. Material candidates are selected based on performance in arc-jet experiments, where materials are exposed to a high temperature plasma plume. While this technique is effective at testing bulk materials and examining them postmortem, it is difficult to couple with in-situ material-specific diagnostics. Lockheed Martin has quoted "material behavior, characterization and response is critically important to developing reliable, predictable and cost-effective flight systems." Thus, complementary in-situ materials diagnostics are required to decouple fundamental material phenomena to better understand core degradation mechanisms to improve hypersonic performance. There are two key techniques that can be used to complement arc-jet experiments: (i) The McCormack lab's environmentally controlled conical nozzle levitator system equipped with dual heating lasers is able to levitate spherical samples in a compositionally controlled gas-stream and achieve temperatures of up to ~4000K. This technique can be coupled with in-situ X-ray powder diffraction to observe temperature effects (thermal expansion, melting, evaporation etc.) as well as chemical reactions in air, while being container-less, which prevents unwanted container reactions. (ii) LLNL is constructing a materials diagnostic wind tunnel that will be operational in 2022, that can achieve hypersonic speeds up to Mach 5 and uses resistive and laser heating to achieve temperatures up to ~4000˚C. In-situ laser-based speckle interferometry and ultrasound testing are incorporated to observe material response, such as thickness, porosity and topology changes. These two systems will be able to decouple material degradation mechanisms for hypersonic candidate materials such as ZrC and HfC in addition to the highest predicted melting point materials, $(Hf_{0.8},Ta_{0.2})C$, Hf-C-N. This study will determine material operation limits, as well as inform the design of next generation barrier coatings and composite systems to further push these materials beyond their current capabilities.

Integrating Model and Data-Driven Methods in IoT-enabled Resilient Infrastructure

Host Campus: Irvine
Lead Investigator: Andrew Chio
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:

My research focuses on applying model-driven and IoT data-driven approaches to enable infrastructure resilience in real-world systems. Today, our infrastructure is becoming progressively strained and fragile. Consider water systems, where aging, increased urbanization, and climate change has increased susceptibility to damage, critically impacting water availability, quality and the ecosystem. Urban structures, e.g. buildings and high-rises, are highly heterogeneous in structure, use and size; energy efficiency, and ensuring safety of occupants during emergencies are critical. Leveraging IoT and AI/ML technologies will be key to the planning, design and operation of next-generation resilient infrastructure.

Our work combines physics-based models with data-driven techniques enabled by sensing/IoT technologies to design tools to aid in better planning and informed decision making for resilient infrastructure. Our experiences have revealed several instances of “inverse” problems, where limited observations from sparse sensing are used to identify potential sources of anomalies, e.g. fault identification in pipeline networks and contamination source identification in drinking water systems, origins of highrise fires. The general setting uses incomplete knowledge of network structures with lossy, real-time data to develop a framework to answer questions such as: Is there an anomalous event in the network? Can we characterize properties of anomalous events and determine its likely source? How can local edge resources be leveraged to provide situation awareness? With people embedded in sensorized spaces, e.g. smart buildings, what is the correct balance between individual privacy and accurate data collection? My research will develop techniques to understand tradeoffs in designing smart infrastructure.

Working with the national labs will allow access to high quality datasets spanning over multiple domains which can serve to validate robustness of models, e.g., to identify and isolate location-specific biases in data. High-performance computing resources at National Labs will be critical in exploring complex algorithms and executing large-scale simulations. Finally, expertise within research labs in areas such as AI-enabled infrastructure resilience will be invaluable in designing meaningful solutions for creating robust and resilient infrastructure for our nation.

Investigation of Productive Binding Sites on Cellulose Towards Improving Biofuel Production

Host Campus: Davis
Lead Investigator: Alex Hitomi
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:

Lignocellulosic biomass exists as an underused and renewable source of sugars that can be fermented into clean, carbon-neutral biofuels. These non-edible plant residues primarily consist of cellulose, a polymer of glucose, which exists within plant cell walls as crystalline fibrils. Efficient conversion of cellulose into biofuels requires not only cellulases, specialized enzymes that degrade cellulose, but also favorable interfacial interactions that facilitate cellulase binding. Recently, cellulose hydrolysis rates were found to be limited by the availability and depletion of productive cellulase binding sites at the fibril surface. For cellobiohydrolase, an industrially-relevant cellulase, these productive binding sites are solvent-accessible cellulose molecules that the enzyme can thread into its active site to perform enzymatic hydrolysis. Biochemical assays of different celluloses over the course of hydrolysis demonstrate that these productive cellulase binding sites deplete as hydrolysis proceeds despite excess cellulose remaining, suggesting that productive binding sites rather than just cellulose are essential for cellulose hydrolysis. Therefore, this work will investigate how to mitigate and prevent productive cellulase binding site depletion on cellulose. Productive binding site depletion depends on both changes to the fibril structure and interfacial properties at the surface of cellulose during hydrolysis, thus nanoscale interrogation of surface properties about binding sites will elucidate both the structure of productive binding sites and their mode of depletion. Preliminary work from our lab with accessory enzyme-treated cellulose demonstrate that changes to fibril surface chemistry increases enzyme accessibility and facilitates cellulose deconstruction. Leveraging complementary imaging capabilities and expanding on existing collaborations between the Center for Integrated Nanotechnologies at the Los Alamos National Laboratory and UC Davis will allow for extensive study of the cellulose surface properties impacting productive cellulase binding and hydrolysis. This research will bridge the understanding between cellulose-cellulase interactions at the nanoscale with mechanistic knowledge of enzyme-driven hydrolysis, establishing the foundation for new pretreatments and protein engineering strategies for efficient biomass conversion processes.

Flow-Directed Electrochemical Rejuvenation of Lithium Ion Batteries

Host Campus: Davis
Lead Investigator: Meghann Ma
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:

The goal of this project is to establish a fluid-based approach for Li-ion battery electrochemical rejuvenation and thus, provide a second life to degraded batteries without expensive pretreatment and separation processes accompanied in current battery recycling methods. Solution-based electrochemical remediation has recently emerged as an effective strategy to increase Li-ion inventory and regenerate the cathodic structure by injecting Li-ions back into a degraded electrode. However, this approach is hindered by a concentration gradient of Li-ions generated from the imposed electric field during intercalation and deintercalation, which results in prolonged treatment durations and low rejuvenation efficiencies. Moreover, few studies have sought to understand and recover the anode, even though cell aging constitutes the degradation of both electrodes. Here, we propose a fluid-based approach to mitigate the formation of concentration gradients of Li-ions near the electrodes to detrap Li-ions from the anode for effective battery rejuvenation. To achieve this, we will design a microfluidic system and validate the release of trapped Li-ions from aged anodes. Then we will design and engineer microflow systems in Li-ion pouch cells to evaluate the proposed technique for commercial Li-ion battery systems. The completion of this study will require facilities in the Materials Science Division including the Li-ion pouch cell assembly facility, electrochemical impedance spectroscopy, and battery testing equipment— all which Jianchao Ye, my primary mentor, specializes in. Congwang Ye will also help with the development of the microfluidic device at the Advanced Manufacturing Laboratory. Their expertise will make this an ideal mentorship to elevate the fundamental electrochemical study to an integrated battery design.

Kinetics of Fusion Plasma Cooling by Frozen Pellets

Host Campus: San Diego
Lead Investigator: Haotian Mao
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:
In a steady-state tokamak reactor, the fusion plasma has a temperature around 10 kilo-electron-volts (keV), which is more than 100 million degrees in Kelvin, and a density at ten to the twenty per cubic meter. This gives rise to an energy density of over 300 kilo-joule per cubic meter. A piece of solid particulate, either accidentally or deliberately introduced into the plasma, would interact violently with the fusion plasma including ablation, rocket force, and ionization/assimilation. Of particular interest is the frozen pellet that would deliver fusion fuel of deuterium and tritium into the core of the fusing plasma, and a mixture of deutrium and high-atomic-number impurities such as neon and argon for disruption mitigation, both of which are envisioned to be essential for the successful operation of ITER as a fusion test reactor. The transformation of atoms from the initial state of a solid particulate to the final state of assimilated electron-ion pairs involves complicated equation of state changes, vapor formation and shielding, and atomic processes that lead to ionization and radiation. A complicating additional factor is the surrounding fusion-grade plasma, which provides the energy source for pellet assimilation into the plasma while simultaneously undergoes aggressive cooling. The most intriguing part is the strong interaction between plasma cooling and material assimilation, which is mediated through the plasma energy flux collected by the frozen pellet through a vapor cloud.

The proposed graduate fellowship would allow a UCSD Doctoral Thesis that performs first-principles simulations of the underlying processes of pellet ablation and vapor shielding in a fusion plasma environment, coupled with the plasma cooling due to the presence of the assimilated pellet materials. This is an outstanding multi-physics and multiscale challenge, but which has a readily available first-principle kinetic description. LANL's VPIC code, with newly enhanced atomic physics capabilities, will be used for the proposed simulation studies. A particularly important innovation here is the deployment of multiple connected VPIC simulation domains and the variable particle marker weights to tackle the strong density variation in plasmas and neutrals, which would otherwise be computationally intractable.

Coccidioidomycosis: Granulomas and Lung Microenvironmental Signals Controlling Infection

Host Campus: Merced
Lead Investigator: Nadia Miranda
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:
Valley fever is caused by unknowingly inhaling the fungal pathogen Coccidioides. Coccidioides grows in the soil as mycelia segments into arthroconidia and when the soil is disrupted and aerosolized, it can be inhaled and cause lung infections. 60% of patients are asymptomatic or display minimal disease. Meanwhile, 40% of symptomatic patients may develop deteriorating health complications for months to years after diagnosis. Clinicians often misdiagnose patients with bacterial infections. Researchers have tried to develop a human vaccine for Valley fever but very little is known about how the fungus interacts with the immune system and the lung microenvironment. There is a critical need to identify which immune cells are interacting with the fungus in the lungs and how these cells control infection. I hypothesize that successful resolution of Coccidioides infection results in memory T cell development in the lungs, where specific T cell phenotypes, interactions, and morphology can be characterized. Aim 1: Discover immunological of murine memory T cells. The immune system develops memory in response to Coccidioides as mice survive repeated reinfections and vaccinations. Although, we do not understand how it does so, what type of memory response it is, and which epigenetic changes occur during memory formation to continue to fight the persistent infection. We will immunize mice to establish memory in vivo and test for immunological memory via surface marker expression and chromatin changes. I hypothesize that protective memory T cells develop in response to Coccidioides infection that express memory T cell markers and localize to the lung. Aim 2: Investigate the lung microenvironment utilizing imaging and computational analysis on human and murine samples. Clinicians and researchers have primarily focused on peripheral blood to analyze the immune system response to Coccidioides. It is poorly understood how the parasitic life cycle works within the lung. Some patients develop granulomas to control the infection, which are understudied across most fungal infections. 10X Visium Spatial Gene Expression Solution is a new technology that will provide spatial information and gene expression data on the same lung samples. I hypothesize imaging granulomas will reveal tissue morphology, heterogeneity, and distinct immune cell interactions during coccidioidomycosis.

Motile Matter: Reconstituting Cell Motility using Osmotic Robots

Host Campus: Davis
Lead Investigator: Pallavi Sambre
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:

Cell motility is pervasive and fundamental aspect of biology. Cells move by positioning their membrane channels to become polar, spending ATP to remodel the cytoskeleton that provides traction for the motion. Cancer cells rely on less traditional pathway to migrate, coupling cell polarity with osmotic energy dissipation. Can we recapitulate cellular motility in synthetic systems? The ability to integrate such energy dissipative, non-equilibrium thermodynamics of living cells in cell-like entities should yield important design principles that pave for entirely new class of self-evolving materials that exhibit life-like characteristics of which cell motility is the earliest step. I plan to reconstitute osmotically driven cell motility in synthetic cell-like, chemo-mechanical robots called giant unilamellar vesicles (GUVs). I hypothesize that GUVs containing asymmetrically distributed membrane water channels like carbon nanotube porins (CNTPs)–developed extensively in Dr. Noy's laboratories at LLNL–when subjected to varying osmolarity, generate directional water fluxes that fuel their vectorial propulsion. Certain amphiphilic lipids mixtures that form the GUVs, separate into coexisting phases. With CNTPs preferentially partitioning within one of the phases, the goal of creating cell-like polar GUVs can be realized. I have organized the project into three aims:1) Prepare and characterize CNTP-containing GUVs that exhibit polarity; 2) demonstrate and quantify directional motions of GUVs in response to local osmotic changes; and 3) explore collective migratory behavior of closely spaced populations of GUVs, which interact via hydrodynamic changes. After identifying lipidic compositions for GUVs that generate polarity, I will employ combination of quantitative characterization tools, like confocal fluorescence microscopy, fluorescence recovery after photobleaching, and time-resolved imaging (all available at UC Davis). Tools like super-resolution microscopy and electron microscopy at LLNL will prove crucial for this project. I will also use innovative microfluidic designs to engineer "tracks" for osmotic motility. Apart from being the first step towards a class of material that communicates with their environment, the project brings together fields, like soft matter, biophysics, and bio-inspired materials that can help in better understanding the "rules of life."

Plant Radiocarbon as an Indicator for Urban Decarbonization

Host Campus: Irvine
Lead Investigator: Cindy Yanez
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2022 *End Date*: 3/31/2024 *Amount*: $ 139,536

Abstract:

Fossil fuel-derived carbon dioxide (FFCO2) emissions constitute 65% of all GHG emissions that force global warming with cities being the dominant contributor (~70%). The expansion of electric vehicle promises significant urban FFCO2 reductions, a big step towards decarbonization and climate change mitigation that demands verification. However, while FFCO2 emissions are well-constrained at the national to global scales, uncertainty is much higher at smaller, policy-relevant scales (i.e. the sub-city level). Advanced remote sensing and in situ networks are monitoring atmospheric CO2 to ensure climate policies are effective. However, it is challenging to infer FFCO2 emissions from its mixing ratio alone because it is smaller than the natural and variable carbon cycle fluxes (i.e. biosphere and ocean exchange).

In the proposed collaboration between UC Irvine and LANL, we aim to assess and enhance the use of plants as passive FFCO2-biomonitors by coupling plant isotopic analysis with new remote sensing and in situ measurements of atmospheric CO2. The radiocarbon (14C, an isotope of carbon with a 5700-year half-life) signature of plant tissue will be used to map fine-scale spatial patterns in FFCO2. Plants growing near FFCO2 emissions are depleted in 14C since fossil fuels characteristically are devoid of 14C. Preliminary analyses showed that annual plant 14C is sensitive enough to detect reduced FFCO2 emissions in California during the COVID-19 pandemic and thus may be a useful tool for monitoring urban decarbonization as climate mitigation policies take effect.

We will determine the extent to which plant 14C can contribute to a better understanding of urban emission sources and evaluate their spatiotemporal sensitivity alongside seasonal measurements of CO2 along an urban-rural gradient. The analysis will elucidate the relationships between land- and atmosphere-based FFCO2 monitoring metrics, and quantify uncertainties regarding the plant 14C approach. Citizen scientists will be recruited to sample plants for 14C analysis in two urban areas: the Los Angeles megacity and the Santiago Metropolitan area in Chile. This project will validate and reveal fine-scale variations in spatial patterns of FFCO2 emissions in urban domes, advance our ability to track emission reductions and support the success of climate change mitigation efforts.

Point Defect and Short Range Order Kinetics in Concentrated Substitutional Alloys

Host Campus: Berkeley
Lead Investigator: Anas Abu-Odeh
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 124,236

Abstract:

Compositionally complex alloys (CCA's), which contain multiple metallic elements with near equal proportions, have garnered much recent attention. These alloys can exhibit desirable combinations of properties, such as strength, toughness and corrosion resistance, which make them attractive for a range of potential applications in energy, transportation and national security sectors. Due to their composition, and the disordered nature of their atomic structure, these alloys display a statistical distribution of local atomic environments that underlie their ability to host a variety of different deformation mechanisms, and that can affect diffusive transport at high temperatures or under irradiation. An important issue for their design then becomes the exact nature of these statistical distributions, i.e., whether they are characteristic of perfectly random compositional disorder, or possess differing degrees of local atomic short-range order (SRO). Understanding the kinetic processes that govern the formation and destruction of SRO is necessary for optimizing properties in the processing of CCAs, as well as controlling their performance in extreme conditions. The proposed scope of this research is to use advanced atomistic computer simulations to investigate these questions surrounding the kinetics of SRO formation and its effect on diffusive transport of relevant point defects. A major limitation with current computer simulation methods at the relevant atomistic length scales is reaching diffusive timescales without simplifying assumptions that limit their accuracy and general applicability. Los Alamos National Lab (LANL) scientists have pioneered the development of a suite of tools to overcome this limitation, called Accelerated Molecular Dynamics (AMD). Working with LANL scientists, AMD methods will be applied to simulate the kinetics of SRO formation, and to understand its impact on point defect diffusion. The work will focus initially on a concentrated Ni-Cr alloy, a material central to LANL's Fundamental Understanding of Transport Under Reactor Extremes (FUTURE) project. Results obtained spanning simulation parameters of temperature, solute, and defect concentration will allow for the development and validation of theoretical models that can predict transport kinetics in systems with SRO, thus opening this analysis to CCA materials more broadly.

Novel image analysis and neural network techniques for observing Earth's surface water dynamics

Host Campus: Los Angeles
Lead Investigator: Bohan Chen
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2021 *End Date*: 3/31/2024 *Amount*: $ 206,496

Abstract:
One of the major hurdles toward developing robust machine learning models for remote sensing image analysis is the difficulty in collecting large amounts of quality training data. This project proposes to tackle this issue by exploring how generative adversarial neural network (GANN) models can be used to maximize the utility of already-existing and often too-small training datasets through novel transfer learning techniques. UCLA Ph.D. student Bohan Chen will undertake dissertation research at LANL, advised by Dr. Jon Schwenk and also Drs. Cristina Garcia-Cardona and Brendt Wohlberg. His Ph.D. advisor, Andrea Bertozzi, has prior joint work with Dr. Garcia-Cardona and has had a prior UC Lab Fees joint research project with Dr. Wohlberg. This is the first time for a joint collaboration between Dr. Schwenk's group and Dr. Bertozzi's group. The GANNs allow us to generate synthetic images by superimposing qualities learned from other images, e.g. adding clouds and noise to existing training data. GANNs will also be used to create additional training data by acting as a translator between sensor types, e.g. transforming cloud-penetrating radar images to Landsat-like optical images. The new machine learning techniques developed will support ongoing work at LANL that seeks to automatically identify surface water from remotely-sensed imagery. Understanding surface water dynamics is crucial for water security, including reservoir monitoring and estimating freshwater abundance. Preliminary research at LANL to detect waterbodies in Landsat imagery shows that a convolutional neural network method outperforms the state of the art Global Surface Water data product. Dr. Schwenk's group has created an abundant high-precision training data set for arctic river waters, but have found that models trained with this data transfer poorly to other regions. Through GANNs and new transfer learning techniques, this project will develop a surface water detection model with a global application based on arctic training data. In addition to data generation, the research will develop hybrid algorithms that combine image segmentation methods with convolutional neural network methods. This project will enable anticipation and mitigation of water security crises via cutting-edge image analysis techniques to estimate water availability without on-the-ground observations.

Scalable Fabrication of Ultra-Strong and Stiff Hierarchical Syntactic Nanofoams

Host Campus: Irvine
Lead Investigator: Cameron Crook
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

Architected materials have garnered intense interest over the past two decades for their desirable combination of otherwise mutually exclusive properties, such as high strength and low density. This is further driven by two recent advances, namely new plate/shell-based lattices with superior properties to beam-based lattices, and the “smaller is stronger” design paradigm, wherein nearly defect-free nano/micro-sized constituent materials enhance strength. As detailed in a recent report on Metamaterials Manufacturing (authored by the mentor, Spadaccini), despite their demonstrated exceptional performance, architected materials have extremely limited industrial penetration, largely due to the lack of scalable manufacturing processes. Furthermore, key high temperature applications require chemical inertness, high strength and stiffness and high temperature resistance, which are mostly associated with undesirably brittle ceramic constituent materials.

We propose to address these two challenges with a research proposal aimed at the introduction, modeling and optimal design of a novel closed-cell architected nanofoam topology with properties approaching the theoretical upper bounds for isotropic materials, and the development of a scalable self-assembly process to produce the aforementioned topology. The proposed topology comprises a hierarchy of micron-sized spherical voids with increasingly small diameter, and will be manufactured by dispersing well controlled hollow alumina spheres in an alumina slurry, producing an ink for direct ink writing (DIW), followed by DIW of hierarchical architected materials with macroscopic geometry and nanoscale-strengthened “constituent materials.” If successful, this work will result in a nanoarchitected ceramic material with exceptional mechanical properties which can be manufactured at the scale and throughput required by structural applications. The proposed research work will capitalize on ink development expertise, DIW equipment, and large area projection and Nanoscribe systems available at the Center for Engineered Materials and Manufacturing at LLNL, in addition to ancillary equipment at the Advanced Manufacturing Laboratory. The dissertation advisor and the lab mentor have been collaborating on a number of initiatives in the area of architected materials for nearly a decade and fully support this application.

Controls of Methane Dynamics in Tropical Peatlands

Host Campus: Los Angeles
Lead Investigator: Alexandra Hedgpeth
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

Rising atmospheric methane (CH4) levels since the early 2000s are likely related to changes in efflux and/or sink strength in terrestrial ecosystems. Much of this increase in atmospheric CH4 has been attributed to greater inter-annual and seasonal variability in climate and water table in tropical wetlands. Tropical ecosystems are projected to undergo large changes in precipitation, which may lead to even larger changes in atmospheric CH4. There are significant gaps in global carbon budgets and climate predictions due to the lack of carbon cycling data from tropical wetlands. Filling in these gaps will help better predict how the large carbon stocks in these soils will respond to future environmental change. The goal of this proposed work will be to assess the environmental controls on methanogenesis and methanotrophy in deep soil profiles across tropical wetland ecosystems where 104 Gt of global carbon is stored. Specifically, we will examine surface and soil profile flux to accurately predict changes in future CH4 efflux. This will be the first assessment of CH4 dynamics in tropical wetlands below 1m, where the majority of CH4 is produced. This project will measure radiocarbon using Accelerator Mass Spectrometry (AMS) to determine source of CH4 from tropical wetlands. The PhD student, Alexandra Hedgpeth, has previously worked at LLNL's Center for AMS and is proficient in sample preparation and graphitization. As such, training will focus on AMS runs, and modeling and interpretation of data under the mentorship of Dr. Karis McFarlane. There is a significant lack of CH4 flux data and a large sampling bias towards Indonesia and Malaysia due to the difficulties associated with field work in these regions. We will conduct the proposed research in a Panamanian wetland site previously established by Alexandra Hedgpeth to add needed data from other tropical wetland regions to provide a more extensive understanding in the spatial pattern of CH4 flux. We hypothesize that the results of this study will demonstrate that in tropical wetlands rapid drops in water table lead to short-lived but large CH4 release from anaerobic subsoils to the atmosphere. We expect that decreased moisture and water table together suppress methanotrophy increasing CH4 efflux.

Interactive Visual Analysis of Data Movement in Heterogeneous Computing Architectures

Host Campus: Davis
Lead Investigator: Suraj P. Kesavan
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

With the end of Moore’s law in sight, High-Performance Computing (HPC) has increasingly focused on heterogeneous architectures to meet the exascale computing goals. Leading supercomputers provide unprecedented capabilities through a combined prowess of large multi-core CPUs and several high-performant GPUs on each computational node. While heterogeneous architectures have demonstrated effectiveness in solving large and complex scientific problems, there still exist many opportunities to improve the returns on investments in this relatively new paradigm.

In particular, although significant speedup can be reaped by porting the computationally expensive operations to the GPUs or by using dedicated I/O nodes, the corresponding data movement costs may substantially compensate for the overall gains. Identification of such data movement penalties, in particular, to and from I/O nodes, between CPUs and GPUs, and across memory hierarchies, can shed new light on the associated bottlenecks, leading to development of new ways to improve the utilization of these architectures.

We propose to develop new visual analysis techniques to enable a detailed investigation of data movement costs and investigate their impact on the application’s performance. We will develop a new framework to allow holistic exploration of data movement to satiate the need for large-scale heterogeneous computing. Focusing on the need for in-situ exploration, e.g., for understanding the data costs of training deep neural networks, we will visualize streaming performance data enabling real-time exploration for applications on heterogeneous machines.

Although one may use known metrics to analyze the performance of applications, such an approach is primarily useful for validating/invalidating their hypothesis. Whereas developing new conjectures about the causes and potential solutions to performance problems is typically not possible. Our framework will inform code developers, computational scientists, and HPC researchers of possible ways to improve machine utilization and efficiently run larger and communication-demanding applications, e.g., by identifying incompatible job placement, and hardware latencies and communication patterns. Overall, our approach can help in narrowing the growing gap between the computing power of processes and data bandwidth at various levels of granularities.

Exciton Transport in 2D and 3D Halide Perovskite Materials

Host Campus: Davis
Lead Investigator: Luke McClintock
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

Excitons have significant effects on the photoinduced response of halide perovskites - materials that promise revolutionary advances in optoelectronic and spintronic technologies. Despite intense efforts, the formation, transport, and spin polarization mechanisms of these excitons are not well understood. My dissertation is focused on understanding exciton behavior in halide perovskites through a wide variety of transport and spectroscopic experimentation coupled to theoretical simulations. Recently, we developed unique fabrication procedures that allow for the novel study of exciton transport under a wide range of temperature and charge density conditions in single crystalline perovskites. We also revealed indirect signatures of excitonic dominance over charge diffusion in perovskites up to technologically relevant temperatures. This Fellowship will allow me to leverage these breakthroughs and visualize exciton dynamics under several key experimental avenues - space, time, spectrum, and dimensionality (3D bulk to 2D molecular layers), with an aim of understanding and manipulating excitonic responses. Through a combination of spatially, temporally, and spectrally resolved temperature-dependent fluorescence and absorption microscopies, we will reveal an increasing excitonic population at low temperatures and provide direct evidence of its connection to enhanced photoinduced carrier diffusion behavior. Furthermore, we will utilize LANL's ultrafast optical microscopy facilities to study the formation and recombination dynamics of the excitons in 2D and 3D samples, thus validating dimensionality as an important tuning parameter for their photovoltaic response. Overall, this work will provide better understanding of the interplay among free carriers, excitons, phonons, and spins and allow us to harness these interactions for creating new materials with enhanced optoelectronic and spintronic properties. Working under joint supervision from Dr. Yarotski (LANL) and Prof. Yu (UCD) will allow me to benefit from their expertise of photovoltaic materials, as well as nanoscale and ultrafast optical and transport techniques. The results of this work will lead to many high-profile publications that will be of great interest to a broad community of researchers in condensed matter physics, optical science, and related fields.

Unraveling the Dark Side of Marine Biotools: Development of Lightweight & Radioprotective Composites

Host Campus: Berkeley
Lead Investigator: Katerina Gensila Malollari
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

In nature, the primary reinforcing elements of structural tissues are almost always inorganic minerals. However, this is not the only blueprint for achieving rigidity, high strength, and abrasion resistance in composites. The Humboldt squid and several carnivorous marine worms have "biotools" (beaks, jaws or teeth) that exhibit impressive mechanical performance yet contain little or no inorganic mineral content. The bloodworm Glycera dibranchiata offers an interesting example, as its load- and impact-resistant jaws are comprised of a network of proteins, mostly unmineralized copper and melanin. The use of melanin as a structural component is a unique design concept not found elsewhere, as the typical biological roles of melanin are pigmentation and photoprotection. Limited prior studies of Glycera jaws revealed hard, strong, and tough mechanical properties- on par with or even exceeding human bone- despite minimal degree of mineralization (<1%). However, the formation of these biocomposites, the exact role of melanin, and the synergy among the various components in the Glycera jaw remain poorly understood. The principal objectives of this research are to elucidate the structure-property relationships of melanin, proteins, and metal building blocks in the jaw and to use this information to inform the design of future lightweight high-performance composites. To unravel this mystery, we will investigate the jaws' molecular and nanoscale mechanics, the morphology and structure of melanin, and the interactions among individual constituents in Glycera jaws by leveraging state-of-the-art 4D scanning transmission electron microscopy (4D-STEM) and single-molecule force spectroscopy (SMFS). In addition, since melanin is known for its extraordinary radioactive shielding properties in organisms exposed to high background radiation levels, we will investigate whether these biocomposites exhibit any radioprotective capabilities. New information regarding the relationship between biochemical structure and mechanical behavior of the various components will be coupled with bioinspired materials processing and the unique capabilities of LLNL on advanced manufacturing processes as well as materials characterization to support the fabrication of biomimetic lightweight yet strong melanin composites, with potential applications as structural and radiation shielding materials.

Probing spin transport in many-body entangled quantum magnets under extreme conditions

Host Campus: Berkeley
Lead Investigator: Vikram Nagarajan
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2024 *Amount*: $ 185,795

Abstract:

The many-body problem is at the root of some of the biggest open questions in physics, including understanding the nature of high-temperature superconductivity, or the fate of quantum information in a black hole. The challenge, simply described, is that the properties of such systems are intrinsically collective and cannot, in general, be framed in the familiar language of a single particle quanta like spin, charge or momentum. Rather, these systems are characterized by emergent quantum numbers which may not take on conventionally quantized values. In this proposal, we suggest a new experimental approach aimed at identifying the underlying characteristics of the collective objects resulting from many-body physics. Our strategy uses state-of-the-art nanofabrication techniques to inject spin into a material, and probe the non-local response carried by these collective objects. Essential to this approach is the ability to tune the system from one many-body state to another, in order to probe the evolution of the collective response. We achieve this by applying extreme pressures, a unique capability developed at Lawrence Livermore National Lab. We focus on a specific class of materials known as quantum spin liquids, a family closely related to high temperature superconductors and theoretically contain emergent spin quanta. Our experiment will reveal how these particles transport information and energy, and demonstrate a path to extending these techniques to answer long standing questions in exotic materials.

A Submerged Wireless Imaging beam Monitor Diagnostic Development for High Rep-Rate Accelerators

Host Campus: Santa Cruz
Lead Investigator: Nora Norvell
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

With the push towards higher rep-rate accelerators to drive particle physics and photon science research, diagnostic systems need to keep up with the influx of signal data as well as be able to withstand increased radiation damage. The guiding goal for this proposal is to develop a profile monitor for these high-repetition machines that can measure pulse by pulse beam metrics such as beam shape, position, bunch length, flux and timing within the pulse train. Knowing these beam metrics is essential to be able to properly tune next-generation X-Ray free electron lasers and particle beam experiments and be able to distinguish what is just an isolated pulse abnormality versus a chronic problem with every pulse. This proposal would generally advance R&D for pulse by pulse, radiation tolerant and effective beam diagnostic profile monitors by specifically focusing on dramatically speeding up and improving how the proton beam at LANL's Isotope Production Facility (IPF) beam line is imaged and tuned. IPF is a critical beam line that produces much of the United States' supply of medical radioisotopes but currently the beam line has a slow and tedious tuning process. I propose to use these fellowship funds to join the Los Alamos Accelerator Operations and Technology group. With Deputy Group Leader Dr. John Smedley, I propose to lead the development of a wireless pulse-by-pulse profile monitor for the IPF beam line. We will design and fabricate a diamond detector to both document the capabilities of diamond detectors on proton beams for pulse by pulse beam characterization as well as significantly speed up the tuning time for IPF. To meet both the needs of the IPF beam line and the diamond detector research community, we propose here a diamond Submerged Wireless Imaging Monitor (SWIM) for the Isotope Production Facility.

The response of Arctic delta morphology and dynamics to permafrost loss and hydrological change

Host Campus: Irvine
Lead Investigator: Lawrence Vulis
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 120,190

Abstract:

River deltas ringing the Arctic Ocean coastline are unique landforms shaped by both highly seasonal cold region hydrology and permafrost features such as thermokarst lakes. These lakes trap, store, and modulate the timing and magnitudes of riverine freshwater, sediment, and nutrients normally routed directly to the ocean through a distributary delta channel network (DCN). Future climate warming is expected to thaw permafrost, modifying lake coverage and therefore riverine flux delivery to the Arctic Ocean, as well as release large quantities of previously frozen carbon into the atmosphere. How and where thermokarst lake coverage on deltas will change, and how these changes will impact sediment and nutrient transport to the coast, remains highly uncertain. We propose a two-pronged approach towards building an understanding of delta lake cover response to warming by: (1) performing a data-driven multiscale analysis of lake sizes and lake and channel network spatial patterns on arctic deltas using satellite imagery and graph theoretic techniques; and (2) developing a simplified modelling approach to project lake cover changes and associated changes to delta riverine fluxes. For (1) we are developing a novel technique to study lake spacing using Voronoi tessellation and then harnessing tools from biology for quantifying multiscale organization of cells in leaves to study the tessellation of lakes on deltas. Our work is expected to discover relationships between lake size and spacing patterns and climate variables which can guide physically-based models upon which future projections can be made. For (2) we will couple a regional thermokarst lake generation model with a reduced complexity model for delta evolution (DeltaRCM), which Dr. Joel Rowland's group at LANL recently introduced ice and permafrost representation into. We will use this to quantify how lake coverage will respond to warming, and how changing lake coverage will modify sediment and nutrient delivery to the coastline. The proposed work builds on an existing NSF Collaborative Project between Prof. Efi Foufoula-Georgiou's group at UCI and Dr. Rowland's group at LANL on analyzing DCN geometry and topology using graph theoretic approaches, and contributes to cross-cutting question #2 of the DOE InteRFACE (Interdisciplinary Research for Arctic Coastal Environments) project of Dr. Rowland at LANL.

Heterogeneous 2D Lamellar Membranes for Improved Separation in Water Purification

Host Campus: Berkeley
Lead Investigator: Monong Wang
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2021 *End Date*: 3/31/2023 *Amount*: $ 139,536

Abstract:

Membrane technology has played a key role addressing global freshwater scarcity, providing additional water supplies such as desalination and water reuse. Lamellar membranes based on homogeneous 2D-materials have demonstrated intriguing performance for water treatment, but suffered from poor selectivity, membrane swelling, stacking defects, or poor stability. To address these problems, I propose to develop heterogenous lamellar membranes by combining Graphene Oxide (GO) with porous nanosheets such as Zeolite and MoS2. Heterogenous stacking of GO-Zeolite/MoS2 nanosheets can minimize membrane swelling by rebalancing the attractive and repulsive forces between layers, thus improving stability of the interlamellar spacing and membrane selectivity. In-plane pores on porous nanosheets and the interlamellar nanochannels provide hybrid transport pathways for molecules, which could be exploited to transcend the permeability-selectivity tradeoff of conventional membrane materials. Together with swelling control, a major goal of my study is to understand the hybrid transport mechanisms in the heterogeneous membranes to achieve high separation performance. I propose to incorporate 2D nanosheets onto a single-nanopore substrate and investigate ion transport using patch clamp technique. This analysis will isolate the molecular transport through in-plane pores and nanochannels by altering substrate pore size and thickness of deposited nanosheets. Molecular transport will be likely dominated by in-plane pores when the substrate pore is small, while transport through nanochannels will be more pronounced with larger substrate pore and thicker nanosheets deposition. TEM-compatible, single-pore silicon nitride membrane will be used as membrane substrate to facilitate device imaging and characterization. This work will leverage the LLNL mentor expertise in nanofluidics and ion/water transport, as well access to LLNL tools for single nanosheet (Axopatch patch clamp and Keithley instruments) and centimeter-scale membrane transport (RO and diffusion cells) characterization. With combined structural and chemical control in 2D membranes and selective characterization of the transport pathways, this research will ultimately provide fundamental knowledge required to develop lamellar membranes meeting the demanding performance metrics for efficient water purification and desalination.

Privacy Risks, Thoughts, Actions, and Regulations

Host Campus: Berkeley
Lead Investigator: Naniette Coleman
Graduate Fellowships
Collaborating Sites: Los Alamos
Start Date: 4/1/2020 *End Date*: 3/31/2023 *Amount*: $200,016

Abstract:

My research examines privacy at the individual and organizational level. The individual focused component interrogates how our personal privacy protection thoughts and actions differ. At the organizational level, my work examines how different organizations assess risk, make decisions, respond to data breaches, and work towards compliance within an increasingly complex web of state, federal, and international privacy laws. The benefits and outcomes of spending 6-months (or more) at Los Alamos National Lab include: 1) thinking more broadly by engaging in unexpected, innovative, interdisciplinary exchanges that expand my theoretical and methodological reach. I expect these will occur every day at the Center for Nonlinear Studies where I have been offered office space should my proposal be selected; 2) digging deeper via hands on work with privacy and cybersecurity content experts who are engaged with the analysis of the exact kinds of data transactions I consider in my work and the creation of IS&T tools. There are, for example, data sharing possibilities between healthcare providers and insurance companies, which will receive greater scrutiny under our new regulatory reality; 3) engaging decisively with my mentor, a statistician who has offered regular consultation as I do battle with the strategic thinking and analytical labor required to thoughtfully process and present findings on the myriad intertwining large data sets I have already collected to answer my research questions; and finally, 4) connecting and building relationships between my new colleagues at LANL and other entities with whom I have formal affiliations (e.g. Berkman Klein Center) for the purposes of expanding our audiences and deepening ties and growing research opportunities. Taking time to reflect is a driving force behind my desire to affiliate with LANL because the outcome of my work on individuals may have workforce implications and my work on organizations may lead to institutional changes. I expect my findings will shift how organizations think about who should have access to private or classified information, what a commitment to guarantee the protection of that information really means, how often that commitment should be reassessed or tested, and how.

Perovskite Quantum Dot Single Photon Emitters

Host Campus: Merced
Lead Investigator: William Delmas
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2020 *End Date*: 3/31/2022 *Amount*: $135,216

Abstract:

With the recent developments in the field of quantum information, it is more important than ever to develop stable and high-quality single photon emitters (SPEs). SPEs are essential for the development of quantum encryption devices, as well as fundamental investigations into quantum mechanical phenomena. In the past decade, several different systems have shown promise as SPEs including defects in diamond, hexagonal boron nitride and several different 2D materials. In addition to the defect-based emitters, quantum dots (QDs) have shown promise as strong SPEs at low temperatures. QD emitters are considerably easier to fabricate and achieve precise placement than defect-based emitters but so far have only worked at cryogenic temperatures. In collaboration with LLNL, we propose to investigate organo-metallic hybrid perovskite QDs as SPEs with the goal of stabilizing their emission through chemical, electromagnetic and plasmonic tuning to make a room temperature SPE. By collaborating with Dr. Ted Laurence at LLNL for his spectroscopy expertise, I hope to gain more insight into advanced time-resolved spectroscopies, such as photon correlation Fourier Spectroscopy techniques, that will measure the quality of our SPEs. We have previously shown that we can chemically tune our QD emission characteristics by changing the ligands that functionalize their surface. In collaborating with LLNL and with Dr. Tiziana Bond, specifically for her expertise in photonic materials as well as in modeling and fabricating plasmonic structures, we hope to use plasmonic structures to increase the SPE emission and tune their spectral properties via plasmonic coupling. LLNL fabrication capabilities with electron beam lithography and gold deposition and their Transmission Electron Microscope for structure characterization will also be of great assistance. The goal of this proposed thesis work is to make advancements in organo-metallic hybrid perovskite QD room temperature SPEs by making strides in our understanding of how to tune and manipulate these devices.

High resolution paleoclimate reconstruction using NanoSIMS

Host Campus: Irvine
Lead Investigator: Kevin Wright
Graduate Fellowships
Collaborating Sites: Lawrence Livermore
Start Date: 4/1/2019 *End Date*: 3/31/2022 *Amount*: $200,016

Abstract:

Variations in precipitation in northeast Mexico can have powerful impacts on agriculture, industry and ecosystems in the region. However, it is uncertain how regional hydroclimate will be affected by climate change due to the short instrumental record and the paucity of paleoclimate records from the region. We propose to utilize geochemical variations in speleothems (cave calcite deposits) collected from NE Mexico, which span the last ~60,000 years, to investigate the timing and mechanisms of past hydrologic change over a range of timescales. Speleothems are unique paleoclimate archives in that they contain multiple climate proxies, can be precisely dated with U-series methods, and can cover seasonal to orbital timescales. The isotopic and elemental composition of speleothem calcite are widely utilized as paleoclimate proxies. However, interpretation is often complicated since multiple processes, from atmospheric to within cave, can influence the geochemical signal. Through collaboration with Dr. Peter Weber, we aim to integrate our long-term speleothem stable isotope and trace element (TE) data collected at UC Irvine, with high-resolution measurements conducted with the NanoSIMS instrument at LLNL, with the goals of improving our understanding of TE incorporation in speleothem calcite, identifying annual lamina for age model constraints, and testing for proxy evidence of extreme hydrologic events, such as droughts and hurricanes. NanoSIMS will allow us to spatially map TEs in key intervals to determine if they are uniformly distributed in calcite or associated with impurities, which has implications for their use as paleo-proxies. The high resolution of SIMS will also allow us to track seasonal changes in speleothem geochemistry, which may reveal annual cycles that could be utilized for age control, as well as for seasonal resolution paleoclimate reconstruction. Finally, annual droughts and extreme precipitation events may not be captured by other analytical methods due to their fast onset and brief duration. High resolution SIMS can potentially be used to identify previously unresolved events and develop new proxies for past tropical cyclones. We will also seek to collaborate with other LLNL scientists on this project, for instance through complementary analyses via SEM/TEM/ICPMS and through seeking collaborations with the E3SM climate modeling groups.

Direct Production of Renewable Fuels and Chemicals from Captured CO2

Host Campus: Davis
Lead Investigator: Louise Berben
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Irvine, Los Angeles, Merced, Riverside, Santa Barbara, Lawrence Berkeley, Lawrence Livermore
Start Date: 3/1/2022 *End Date*: 2/28/2025 *Amount*: $ 3,750,008

Abstract:

Electrochemical approaches enable conversion of renewably-derived electricity into chemicals and fuels, and can be used to recycle CO2 and advance decarbonization technologies. This center will pursue fundamental discoveries in reaction chemistry and catalysis that will open access to useful chemical and fuel products that were previously inaccessible using CO2 as substrate. Reactive capture of CO2 will directly combine the capture of CO2 with conversion of captured CO2 into value-added products; and significantly improve the cost and overall efficiency relative to current standard multi-step processes. Reactive capture of CO2 offers the ability not only to clean up underutilized or dirty CO2 from waste streams, but also provides a mechanism to tune the reactivity of CO2 as substrate by variation of the capture reagent. This center bridges fundamental and applied work by combining the development of new molecular and heterogeneous electrocatalyst systems with reactor design and engineering that will enable prototyping electrocatalytic reactive capture of CO2 beyond the proof-of concept stage. We will also establish a record of collaborations between UC, LLNL and LBNL that facilitates finding extramural funding.

We will address the ambitious goals with a synergistic center approach that leverages the strengths of UC, LLNL, and LBNL PIs, by combining experimental and theoretical expertise in thermal catalysis and molecular and heterogeneous electrocatalysis with reactor design and reactor modelling for scale-up. Experiments and theory will both contribute to the design new catalysts, model active sites, mechanisms and pathways for molecular and heterogeneous electrocatalysts from first principles; including the experimental conditions, such as solvent, and applied potential. Advanced manufacturing expertise at LLNL, led by Drs. Eric Duoss and Christopher Hahn, will enable rapid prototyping of components and reactors to integrate fundamental electrochemical processes for reactive CO2 capture into sub-scale systems where reactive CO2 capture is paired with a useful, established oxidation process to maximize efficiency. Expertise at LBNL, led by Dr. Adam Weber, will enable design and optimization of the CO2 reactive capture cell through multiphysics modeling of the phenomena within the cell.

California's Deep Decarbonization Pathways: A Holistic Multi-Layer Assessment

Host Campus: Los Angeles
Lead Investigator: Rajit Gadh
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Merced, Riverside, Lawrence Berkeley, Lawrence Livermore
Start Date: 3/1/2022 *End Date*: 2/28/2025 *Amount*: $ 3,898,891

Abstract:

California, as the world's fifth largest economy, has been a global leader in setting aggressive climate and decarbonization goals. The recently published SB100 Joint Agency Report suggests that California's ambitious carbon neutrality goal by 2045 is technically achievable through multiple pathways, and the remaining challenges lie in the scale and speed of accomplishing this goal. It is critical to holistically assess existing technological readiness, supporting policies, and legislative frameworks and fill in the gap of existing pathway scenarios across sectors. To this end, we propose a new multi-layer holistic assessment of California's deep decarbonization pathways and synthesis of key technology and deployment gaps as well as supporting policies needed for California to meet the 2045 goal of carbon neutrality. The study will involve multiple sectors - including transportation, electricity, and buildings - and will consider the cross-sector interdependencies, climate change impact and the emerging environmental justice concerns to fill in the gap of the existing emission reduction pathways. This interdisciplinary effort will build multi-layer decarbonization pathway scenarios and perform cross-sector simulation evaluations at multiple temporal and spatial scales, based on which the policy implications will be derived to support emission regulations and new policy changes. The team will also leverage their expertise on artificial intelligence (AI) to identify AI potentials on improving the speed and scope of decarbonization pathways. The team consists of multiple UC campuses: UCLA, UC Riverside, UC Berkeley, UC Merced, and two national laboratories, Lawrence Berkeley National Laboratory (LBNL) and Lawrence Livermore National Laboratory (LLNL). The project will combine a wealth of educational and mentoring activities across a diverse team of undergraduate and graduate students and postdoctoral scholars on 4 UC campuses, as well as access to Lawrence Livermore National Lab and Lawrence Berkeley National Lab's testbeds and high-performance computing resources. The proposed framework will provide publishable data and a knowledge base for students and postdocs and will engage professionals to develop and test new tools, advancing decarbonization and accelerating the adoption of emission reduction technologies.

Multiscale Interaction and Inverse Design of Metallic Meso-architected Materials for Dynamics

Host Campus: San Diego
Lead Investigator: H Alicia Kim
Collaborative Research and Training Awards
Collaborating Sites: Irvine, Santa Barbara, Los Alamos, Lawrence Livermore
Start Date: 3/1/2022 *End Date*: 2/28/2025 *Amount*: $ 3,728,321

Abstract:

Recent advances in additive manufacturing (AM) enable exquisite control over the meso-scale (microns to tens of centimeters) unit cell topology of architected materials. Yet our ability to design for desired performance is currently limited to the simplest linear phenomena, e.g., linear elasticity, thermal conduction, permeability. The development of experimentally verified, physics-based, efficient computational methods for optimal design of meso-architected materials in the high-strain rate conditions of interest to LLNL and LANL would be transformational for applications such as blast and penetration mitigation.

We identify two major challenges in tailoring the dynamic behavior of AM meso-architected materials. First, the material properties of the solid vary as a function of microstructural features (finer than the mesoscale lattice geometry) due to local processing conditions. Coupling between micro- and mesoscale features poses unique challenges in modeling and design. Second, the dynamic response of two-phase materials is highly complex with many nonlinearities, e.g. plasticity, fracture, fluid structure interaction, shock propagation.

We will address the challenges by bringing together a diverse team of multidisciplinary experts: Kim (multiscale optimal design, UCSD); Boechler (nonlinear dynamics of meso- architected materials, UCSD), Valdevit (AM fabrication and characterization of meso-architected materials, UCI); Begley (nonlinear metamaterials, UCSB); Spadaccini (advanced manufacturing, LLNL); Hunter/Fensin (impact systems, LANL). Focusing on nonlinearities relevant to weak-shocks in ductile metals, we will develop low-cost computational models, create an inverse design framework to generate optimal micro- and meso-architected materials, and validate experimentally. This project will strongly rely on unique facilities at LLNL and LANL: NNSA's Dynamic Compression Sector at the Advanced Photon Source and other dynamic testing facilities, the high-performance computing capabilities and codes, and advanced manufacturing including the Advanced Manufacturing Laboratory at LLNL. We expect the impact on scholarship to be substantial across many disciplines: materials, mechanics, manufacturing, numerical analysis and digital engineering. The budget of $1.25M/year will support $330K to UCSD (Kim and Boechler) and $230K each to UCI, UCSB, LANL and LLNL.

Improving pandemic preparedness and health equity through wastewater-based epidemiology

Host Campus: Berkeley
Lead Investigator: Kara Nelson
Collaborative Research and Training Awards
Collaborating Sites: Davis, San Francisco, Lawrence Livermore
Start Date: 3/1/2022 *End Date*: 2/28/2025 *Amount*: $ 3,920,170

Abstract:

Wastewater-based epidemiology (WBE), the tracking of pathogens and biomarkers in sewage to inform public health, has rapidly become widespread during the COVID-19 pandemic. While clinical testing is biased toward symptomatic individuals with access to health care, wastewater testing provides a comprehensive picture of disease prevalence in geographically constrained regions. Both the difficulties of conducting wastewater testing and the benefits of WBE encountered during the COVID-19 pandemic highlight the need to hone this tool in preparation for future pandemics. Here we propose to conduct 1) a comprehensive analysis of COVID-19 data that integrates wastewater testing, 2) rigorous methods development and benchmarking for variant- and strain-level identification and quantification of respiratory viruses in sewage, and 3) application of these methods to collect new data on the epidemiological patterns of respiratory viruses in Northern California. The field of WBE is highly interdisciplinary, involving environmental engineers, microbiologists, epidemiologists, and public health researchers. Hence, our effort will include interdisciplinary training of students and postdoctoral scholars within a collaborative team from U.C. Berkeley, U.C. Davis, U.C. San Francisco, and Lawrence Livermore National Laboratory (LLNL). LLNL has recently developed techniques that have the potential to advance the field of WBE, including assays of virus viability from environmental samples, protein-based detection of mutations for samples lacking intact nucleic acids, and software to design custom DNA sequencing panels targeting novel strains of pathogens. Students and early-career scientists will have the opportunity to learn these techniques, adapting them for WBE.

Potential impacts of WBE research on pandemic preparedness are many. In particular, improved wastewater testing could provide early warning of new viral strains or variants before they appear in clinical settings. Finally, because wastewater captures populations that may be difficult to reach by clinical testing, WBE has the potential to address critical questions of health equity, improving pandemic response for all.

Coastal Wetland Restoration: A Nature Based Decarbonization Multi-Benefit Climate Mitigation Solution

Host Campus: Santa Cruz
Lead Investigator: Adina Paytan
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Davis, Irvine, Santa Barbara, Lawrence Berkeley, Lawrence Livermore, Los Alamos
Start Date: 3/1/2022 *End Date*: 2/28/2025 *Amount*: $ 3,645,821

Abstract:

This cross-disciplinary research collaboration aims at advancing decarbonization by assessing carbon sequestration potential and economic value of nature-based coastal blue carbon sequestration in wetlands and identifying management and policy approaches local and regional governments can use that prioritize coastal wetland restoration and conservation projects as a viable solution for combating climate change and mitigating its impacts. Nature based solutions have recently been identified as high priority implementation targets in the USA (Biden climate-plan - helping leverage natural climate solutions by conserving 30% of America's lands and waters by 2030) and worldwide. These solutions provide multiple benefits (flood protection, jobs, food, equity, biodiversity, recreation) including climate mitigation (Griscom et al., 2017). The project will include physical, biological, economic, and social science aspects as well as field and lab work and climate ecosystem and modeling, data science, and education components. It will integrate environmental justice considerations, policy, and governance approaches to develop a framework and guidelines for incorporating coastal wetland restoration/conservation into long-term national adaptation and development plans, facilitating the inclusion of coastal wetland restoration/conservation in carbon credit markets to combat climate change while considering multiple co-benefits (e.g., developing local and regional plans, funding, permitting, leveraging science, political leadership, and community engagement). Harnessing nature-based solutions that also offer adaptation opportunities and enhance community resilience and environmental justice is key to safeguard livelihoods in the face of climate change.

Our multidisciplinary team will work collaboratively to integrate all aspects of the project, but PIs will have clear and distinct responsibilities based on their expertise. We will coordinate tasks in advance and have monthly all participant virtual meetings and annual in-person meeting. Our team includes faculty and researchers at all career stages from undergraduate students to senior scientists, providing opportunity for mentoring and professional development. A new undergraduate course focused on climate data literacy using authentic data will be developed and offered at all participating campuses.

Topological materials for Majorana-based quantum information

Host Campus: San Diego
Lead Investigator: Monica Allen
Collaborative Research and Training Awards
Collaborating Sites: Davis, Los Angeles, Santa Barbara, Los Alamos
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,440,222

Abstract:

Topological materials offer a route to circumvent environmental perturbations that have hindered the scalability of conventional quantum computing architectures. The Majorana mode, which can be artificially engineered in hybrid devices that couple superconductors with topological materials, constitutes a key building block for a fault-tolerant quantum computer. Manipulation of such particles in complex device networks could enable a more robust paradigm for quantum information. We propose a comprehensive, multi-disciplinary program to synthesize and characterize an emerging class of topological superconducting materials posited to host Majorana modes. The overarching goal is to understand the fundamental physics while evaluating the feasibility of prototype devices that may enable braiding of particles in two dimensions. This program will leverage the broad expertise of a diverse team of scientists in materials synthesis, microscopy, device nanofabrication, quantum electronic transport, unconventional superconductivity, and high magnetic field measurements. It consists of three main research thrusts: (1) prediction and synthesis of emerging quantum materials, (2) characterization of topological phases and emergent phenomena in exotic superconductors and other platforms for Majorana modes, and (3) local interrogation and manipulation of topological states in mesoscopic devices. Bulk crystals and thin films will be synthesized at UCSB, UCD, and LANL, and state-of-the-art epitaxy of superconducting films on semiconductor materials will enable production of hybrid material systems with unprecedented interface quality. Upon integration of the materials into device structures, an array of quantum transport measurements will be performed to unequivocally identify Majorana modes, including tunneling spectroscopy and superconducting interferometry. To complement these efforts, we will employ milliKelvin microwave impedance microscopy measurements to achieve the first real-space visualization of Majorana modes in devices. The proposed work will lay the groundwork for the creation of scalable networks of devices for Majorana-based quantum computation. Graduate students and postdoctoral fellows will benefit from training on state-of-the-art facilities and collaborations at LANL, and periodic meetings will bring together scientists across career stages.

Transforming prescribed fire practices for California

Host Campus: Irvine
Lead Investigator: Tirtha Banerjee
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Riverside, Los Alamos
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,600,000

Abstract:

Widespread recognition of the importance of low intensity fires to reduce the frequency and severity of future megafires has prompted California to allocate more than $1 billion over the next five years to support prescribed fire (Rxfire) activities. However, several factors limit Rxfire usage at sufficient scales to effectively minimize the risk of future catastrophic fires: e.g. narrow burn windows, air quality concerns, public perception, personnel training, and liability constraints. To address these urgent needs, our interdisciplinary team will develop technological and operational tools to facilitate the expansion of Rxfire in CA. Our effort will leverage unique multi-fidelity wildfire modeling capabilities, FIRETEC and QUIC-Fire, to assess the effects of (1) heterogeneous fuel structure on fire and smoke behavior; (2) CA and site-specific complex topography, flammable vegetation, micrometeorology and wind patterns; (3) novel ignition strategies e.g., aerial ignitions; (4) complex wildland-urban interface; (5) extents of pollutant formation and transport. Moreover, we will develop technologies/tools that can facilitate communities' understanding of Rxfire. Model ensembles will be aided and calibrated by sensors (in situ and mobile) that capture air quality, visibility, smoke, acoustic signatures, and imagery/video; while UAVs equipped with LIDAR and thermal cameras can further guide sensing. This information in conjunction with community crowdsensing will help map fuels at fine resolutions, monitor Rxfire progress, detect hotspots and quantify community impact. The use of data analytics and machine learning techniques trained by models on real time sensor data will help manage uncertainty in data, detect anomalous behavior rapidly, identify the source locations and potential abort points. The decision support and operational tools will be tested during actual Rxfires in collaboration with US Forest Service, Cal Fire and UC ANR, thus providing publishable data, training for students and postdocs as well as engaging fire practice professionals to develop and test the new tools. The multi-fidelity approach will foster collaborations between UC Irvine (fire modeling, IT decision support), UC Riverside (smoke chemistry and transport), UC Berkeley (experimental Rxfire operations at Berkeley forests) and LANL (model development, high performance computing).

Assessment and mitigation of wildfire-induced air pollution

Host Campus: Davis
Lead Investigator: Michele Barbato
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Irvine, Los Angeles, Merced, Lawrence Livermore, Los Alamos
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,749,855

Abstract:

Wildfire smoke threatens the health and quality of life of millions of people (especially Californians) every year. We propose an innovative, scalable framework for assessment and mitigation of wildfire-induced air pollution under climate change. For the first time, we will develop wildfire forecast tools that link statistically-based regional forecasts spanning multiple decades with short-term physics-based fire propagation models that can accurately forecast individual wildfires. Our innovative approach will predict fuel loads using a semi-dynamic vegetation ecology model in order to estimate future wildfire emissions. Emissions of potentially harmful wildfire particulates will be characterized through laboratory tests of mixed fuel loads (i.e., forest and buildings) typically found in the wildland-urban interface. The results of these experiments will inform: 1) new models of smoke plume transport and chemical transformation, which will be validated using satellite imagery; and 2) a novel high-throughput screening method to assess wildfire smoke toxicity. The toxicological study results will inform epidemiological analyses to estimate the association of wildfire smoke on human health. The health effects of four distinct mitigation strategies (i.e., urban growth policy, vegetation management, prescribed burns, and use of fireproof building materials) will be assessed in conjunction with issues of policy design, regulatory assessments, program monitoring/evaluation, financial feasibility, and social impact. Finally, the project results will be made public on the Cal-Adapt web platform. The proposed research activities will: 1) leverage the strengths of 5 UC campuses and 2 national labs; 2) engage multiple faculty, postdocs, and graduate students across disciplines in mutually beneficial new collaborations; 3) position our team members as international leaders on a timely topic of critical importance with significant potential for extramural funding; and 4) produce considerable societal benefits. This project will support valuable training/exchanges of students/postdocs among collaborating institutions, and structured mentorship/professional development activities for early career UC faculty and lab researchers. Finally, the Electric Power Research Institute plans to collaborate on this project and provide internship opportunities for student training.

Enabling Scalable Quantum Computing

Host Campus: Riverside
Lead Investigator: Boerge Hemmerling
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Los Angeles, Santa Barbara, Lawrence Livermore
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,750,000

Abstract:

Quantum computing is poised to drive the next technological revolution. Driven by the need of system integration and scalability today's quantum computing processors are based on 2D architectures. However, the 2D approach comes at the cost of increased gate errors and reduced connectivity. Here we break with this paradigm and propose to leverage novel 3D printing capabilities with sub-micrometer resolution to develop a scalable 3D-architecture based on trapped ions that will enable extensive quantum calculations with thousands of qubits in the near future. Implementations using traditional 3D Paul traps have already demonstrated memory times of several minutes, extremely low gate errors, and advanced quantum calculations. Moving to a scalable 3D-geometry will increase the confinement by about a factor of three to six and create traps up to 100 times deeper than what is feasible with 2D-fabrication. This is expected to reduce multi-qubit gate error rates by more than an order of magnitude. These advances will also enable novel approaches to quantum computing such as using trapped electrons or molecules, which share the same advantages as trapped atomic ions, while reducing the optical technology overhead. For this research program, we plan to leverage the existing infrastructure and expertise in two-photon 3D-printing and materials science at LLNL and combine that with world-leading expertise in ion-trap quantum information systems within the UC system. Groups at UCLA and UCB have established efforts in trapped-ion quantum computing, with demonstrations of the highest-fidelity single qubit, deep experience with multi-qubit entangling gates and the materials issues related to scalability. Groups at UCSB and UCR have extensive experience in microwave engineering, cryogenics and quantum simulation and work on establishing qubits based on molecules. Through this project, we will design, simulate, and test miniature scalable traps fabricated using 3D-printing methods and show their superior performance compared to current microfabricated traps. We anticipate record-setting error rates, long ion lifetimes and a path to scalability for quantum computing. If successful, this project will solve the most important problem of the scalability of quantum computing architectures and transform the field of quantum information science from within the UC system.

Mitigating and Managing Extreme Wildfire Risk in California

Host Campus: Santa Barbara
Lead Investigator: Charles Jones
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, San Diego, Lawrence Berkeley, Lawrence Livermore
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,307,845

Abstract:

The recent tragic examples of wildfires in California underscore the importance of understanding the relationships among climate, extreme fire-weather, fire ignitions by electric powerlines and vegetation management. This proposal assembles a multidisciplinary team to investigate the interactions among four research themes —climate change and fire-weather, vegetation management, the electric power grid and associated policies — and their influences on wildfires. To make groundbreaking discoveries, this proposal will investigate a series of critical questions: what is the nature of changes in extreme fire-weather behavior in recent years? What factors interact with electric power system infrastructure to increase wildfire risk in California? How do trade-offs between reliability of energy supply and wildfire risk vary across alternative de-energizing protocols? Can cost-effective investments be implemented in the near future to minimize fire-risk associated with vegetation management and electric power grid infrastructure? The project consists of five interconnected objectives that will foster collaborations among 3 UC campuses and 2 national labs. Objective-1 will use a broad array of observations, global and regional climate models to investigate the problem of climate change and potential changes in fire-weather regimes in California. Objective-2 will use the unique database of high-resolution fire-weather regimes (Objective-1) to determine fire-risks associated with high winds and electric powerlines ignitions. Objective-3 will develop a model of de-energization rules applicable to the electric power grid under high winds and re-estimate fire-weather risk. Objective 4 will evaluate the reliability implications of alternative de-energization rules and contrast these with estimates of the economic impacts of mitigating increased fire risks (Objective 2). Objective-5 will analyze observations and model simulations to determine fire-spread and economic impacts of vegetation management strategies near power lines. The project will combine a wealth of educational and mentoring activities across an innovative and diverse team of undergraduate and graduate students, and postdoctoral scholars on four UC campuses.

Advanced Detectors for XFELs and Proton Accelerators

Host Campus: Davis
Lead Investigator: Eric Prebys
Collaborative Research and Training Awards
Collaborating Sites: Irvine, Santa Barbara, Santa Cruz, Lawrence Berkeley, Los Alamos
Start Date: 3/1/2020 *End Date*: 2/28/2023 *Amount*: $3,745,225

Abstract:

As accelerator laboratories around the world aspire to create beams with ever-increasing repetition rate and intensity, there is a need to develop fast, radiation-hard detection technologies to provide critical real-time beam diagnostics. Los Alamos National Laboratory (LANL) is engaged in multiple accelerator (proton and photon) projects to meet mission needs, including those which require diagnostic capability beyond the current state-of-the-art. Solid-state sensors, such as those based on diamond and silicon, feature fast saturated drift velocities and collection dynamics that make them natural choices to explore for development of high-speed devices. In addition to these “front end” technologies, it will be essential to develop highly-granular high-speed electronics – for both amplification and data-handling – to achieve the required spatial and temporal precision. This project will bring together expertise in accelerator and high-energy physics sensor development with electrical engineering expertise to develop prototype systems at the forefront of accelerator beam detection technology. The collaboration will be led by Eric Prebys, Director of the Crocker Nuclear Laboratory at UC Davis, and consist of three interrelated thrusts: R&D on diamond sensors (primarily LANL and UC Davis), silicon diode sensors (primarily UCSC and UCSB) and enabling electronics and readout (primarily UC Irvine and LBNL). However, as each institution has broad expertise in instrumentation development and specialized capabilities in sensor fabrication and readout development, all six institutions will contribute in some measure to all three areas. Crocker Lab and LANL also provide accelerator (cyclotron, LANSCE) facilities well-suited to the validation and characterization of the prototype detection systems developed by the collaboration. UC students will be involved in design, fabrication, testing and data analysis aspects of the project, and will be provided an opportunity to spend a period of time in residence at LANL. Project progress will be disseminated through seminars at member institutions, workshops, presentations at national and international conferences and publications. The project will create strong collaborative ties (both intra-UC and UC-LANL) that well position the group to establish leadership in the area of advanced detection technologies for accelerators.

Great Power Competition in the 21st Century

Host Campus: San Diego
Lead Investigator: Tai Ming Cheung
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Irvine, Los Angeles, Lawrence Livermore
Start Date: 3/1/2018 *End Date*: 2/28/2021 *Amount*: $3,724,742

Abstract:

Great power strategic competition has returned to the global stage and the consequences for international peace, stability, and prosperity will be profound. The contours, dynamics, and characteristics of this new strategic rivalry, primarily between the U.S., China, and Russia, but also to a lesser extent with other emerging power centers, will be very different though to what took place in the 20th Century. Confrontation will not be through massed armies in Europe or nuclear arsenals on trigger alert but will occur more indirectly and in more non-military domains. Strategic rivalry is taking place in the pursuit of technological innovation, in disputes below the threshold of full-scale war, and in trade, investment, industrial, and economic competition. This project examines the rise of 21st Century great power competition that is especially focused on the intersection between economics, strategy, security, technology, and politics. The project revolves around four themes each led by a University of California (UC) campus: 1) competition in security, technology, innovation, and strategy (UC San Diego); 2) economic strategic rivalry in trade, investment, and industrial policy (UC Berkeley); 3) the role of design and production networks in East Asia's regional relations and US-China cooperation and competition (UC Irvine); and 4) the international dynamics and domestic politics of great power security competition (UC Los Angeles). This project brings together scholars from political science, international relations, security studies, political economy, and area studies from these four UC campuses as well as Lawrence Livermore National Laboratory. While scholarship on great power competition is beginning to emerge, much of the work is on military, diplomatic, and hard power aspects and little attention has so far been paid to the technological, economic, and domestic dynamics. Opportunities for students to participate in collaborative research and training activities include: 1) the ability to take part in research teams that will write conference papers; and 2) taking part in a summer training workshop on great power competition that will be conducted in the second and third years that will examine the security, economic, political, and geostrategic dimensions of great power competition.

Headwaters to groundwater: Resources in a changing climate

Host Campus: Santa Barbara
Lead Investigator: Jeff Dozier
Collaborative Research and Training Awards
Collaborating Sites: Davis, Irvine, Los Angeles, Merced, Lawrence Berkeley, Lawrence Livermore
Start Date: 3/1/2018 *End Date*: 2/28/2021 *Amount*: $3,716,025

Abstract:

Climate change and greater water demand pose new challenges for managing water resources. To enable California to optimize future water infrastructure, legislation, and economy, scientists at 5 UC campuses, LLNL, and LBL will measure and model water from headwaters in the Sierra Nevada, through rivers, reservoirs, and groundwater in the Central Valley. The approach is to examine hydrologic sensitivities to changing climate and water demand through models and the historical record. The goal is to provide information to optimize water storage, quality, and groundwater sustainability as precipitation varies, temperatures warm, and population grows. To consider the range of headwater-to-groundwater systems, we focus on three river basins comprising different climatic, geologic, and socio-economic settings -- Shasta R (volcanic, northernmost, lowest, wettest), Kings R (granitic, southernmost, driest, highest, poorest), and the American R (metamorphic, wealthiest). Novel methods to monitor and model ongoing and future changes in rain and snowmelt in the headwaters will be coupled with process-driven modeling and measurement of evapotranspiration, groundwater recharge, and withdrawal in the lowlands. Models will consider changes in water policy and infrastructure, and resulting impacts on energy production and consumption. Collaboration between the Campuses and Labs will build teams that include people in all career stages who study aspects of the water cycle from remote sensing of snow to water policy. Collaborators from LLNL and LBL contribute expertise in isotopic tracing of water, high-performance computer modeling of groundwater and surface water, and energy implications of water management. This proposal strengthens DOE’s mission, to ensure America's security and prosperity by addressing energy, environmental, and nuclear challenges through science and technology. The alliance between UC faculty, postdoctoral fellows, and students with scientists at LLNL and LBL will improve understanding of how changing climate and water demand will affect water resources through the middle to the end of this century. Our proposal will nurture a generation of scientists in the nexus of climate, water, and energy. An advisory board of water practitioners will help target our findings to help water managers make the best decisions for California’s precious water resources.

The Future of California Drought, Fire, and Forest Dieback

Host Campus: Los Angeles
Lead Investigator: Alex Hall
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Davis, Irvine, Lawrence Berkeley, Los Alamos, UC Division of Agriculture and Natural Resources
Start Date: 3/1/2018 *End Date*: 2/28/2021 *Amount*: $3,681,721

Abstract:

From 2011 to 2015, California experienced a drought of historic severity, due to a persistent precipitation deficit and extreme warmth. The drought was bracketed by two extremely wet years in 2010 and 2016, and was accompanied by unprecedented tree mortality and wildfire in California's wildlands. Over the 21st century, climate scientists predict continued warming and an increase in swings between extremely wet and dry conditions. Since wet conditions favor vegetation regrowth and fuels buildup, and warm, dry conditions favor forest dieback and wildfire, these predictions raise questions critical for California's future: Are the extreme forest dieback and fire conditions seen during the recent drought a harbinger of even greater future changes? What do future changes mean for California's unique ecosystems, forest and fire management practices, and economy? Here we propose an effort to answer these questions through collaboration among climate scientists, satellite experts, vegetation modelers, fire scientists, and ecologists. The project will be grounded in analysis of observed relationships between fire, tree mortality, and climatic conditions during the recent drought. We will then develop computer simulations of climate, vegetation, and fire to determine the causes of recent tree mortality and fire variations. We will quantify the role of recent climate change in worsening the observed forest dieback and fire. The project's capstone will be high-resolution climate change projections to simulate the impact of warming and increases in precipitation extremes on 21st century vegetation growth, fire, and forest dieback. We will also assess how future forest and fire management might evolve to mitigate the largest impacts of climate change on California's wildlands. The first-of-their-kind climate, vegetation, and fire simulations will deepen our understanding of the complex interactions within California's wildlands, and will leave a technological legacy in the form of a modeling framework that is easily applied to other regions. The research process will train young scientists in societally relevant interdisciplinary research, the results will help stakeholders plan effective climate change adaptation and mitigation, and our outreach efforts will educate the public about climate change impacts on the treasured lands and resources they depend on.

Climate Impact of Manure Management from California Dairies

Host Campus: Riverside
Lead Investigator: Francesca Hopkins
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, Davis, Irvine, Lawrence Berkeley, Los Alamos
Start Date: 3/1/2018 *End Date*: 2/28/2021 *Amount*: $3,839,477

Abstract:

Climate Impact of Manure Management from California Dairies The California dairy industry is a large contributor to greenhouse gas emissions, producing approximately 50% of methane (CH4) and 10% of nitrous oxide (N2O) emissions statewide. The majority of these emissions come from manure, where emission rates are thought to differ greatly among different manure management techniques. In order to fulfill statewide emission reduction goals for short-lived climate pollutants, the California Air Resources Board has recently targeted CH4 emission sources for near-term mitigation. However, few studies of CH4 emissions from dairy manure have been performed in California. Recent top-down atmospheric observations and inverse model analyses of atmospheric CH4 and N2O levels in the San Joaquin Valley suggest that emissions from dairy agriculture are underestimated in the state inventory. However, the dearth of California-specific information leads to uncertainty in the state inventory that poses an obstacle to efficient, well-informed mitigation planning for emissions from this sector. In addition, the efficacy of proposed mitigation solutions, such as anerobic digesters for manure waste, is not well quantified or tested in practice. We propose to combine top-down atmospheric methods with bottom-up process-level measurements and operational insight to improve both facility specific and regionally integrated estimates of greenhouse gas emissions from management practices at California dairies. Using a unique combination of subject area knowledge, high resolution data sets, biogeochemistry, atmospheric composition observations, and inversion modeling, we will quantify and apportion CH4 and N2O emissions to their sources with the goal of improving understanding of the driving processes and their respective control techniques. By working across scales, we will provide an integrated regional emissions estimate with sufficient detail to unambiguously quantify dairy livestock emissions as distinct from other greenhouse gas sources. This study will give a thorough scientific treatment to the greenhouse gas emissions from the entire manure management cycle in ways that have been done for other CH4 emitting sectors, such as natural gas, to enable complete, empirically informed mitigation decisions.

Political Conflict and Stability in Dynamic Networks

Host Campus: Los Angeles
Lead Investigator: Arthur Stein
Collaborative Research and Training Awards
Collaborating Sites: Berkeley, San Diego, Santa Barbara, Los Alamos
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Abstract:

At the heart of international politics are the cooperative and conflictual relations between states and rebel and terrorist groups. Challenges and opportunities for bilateral ties are posed by their being embedded in a larger setting. The proverb “the enemy of my enemy is my friend” captures this dynamic in which links between pairs of actors are affected by the relationships of each with others. This has huge consequences for interstate and intra-state relations and for critical security questions such as the impact of foreign intervention, or the reverberating impact of a change in international alignment. These relationships constitute a network whose instabilities and dynamics are not well understood. We propose applying to such political relationships a sociological theory (structural balance) developed for networks of interpersonal relationships. The theory requires both analytic development and empirical assessment. The theory originally dichotomized relationships into positive and negative, but we will incorporate the consequences of degrees of cooperation and conflict. The theory stipulates conditions of balance and equilibrium, but does not delineate the specific relationships that will change to bring any set of unbalanced relationships into balance. This will be an analytic extension developed in the project. The empirical assessment of the behavioral dynamics of structural balance will make use of a database of political events, that includes both states and rebel groups, and that codes cooperation and conflict. In addition, surveys and survey experiments will be used to assess the issues and attitudes that underlie structural balance in conflict and post-conflict settings. The project addresses key security concerns, among them being the foreign policy implications of regime change, the reverberating consequences of an outbreak of a civil war or conversely of a peace agreement, and the consequence of an external intervention into a domestic dispute. More broadly, the general model developed of networks of cooperative and conflictual ties will have broader implications for studying political and social relationships. The proposal brings together political scientists who have focused on international and civil conflict with sociologists and applied mathematicians who have worked to develop, assess, and apply networks.