Research Project #1

**Title:** Predictive Computational Catalysis: From Electrons to Reactors

**Principal Investigator:** Steven H. Overbury, Chemical Sciences Division and Center for Nanophase Materials Sciences, overburysh@ornl.gov, 865-574-5040.

**Project Description:** Our overall goal is to create a new computational methodology for a predictive description of catalysis through the integration of atomic simulations with meso- and macroscopic models, thereby, enabling control of catalysis with unprecedented fidelity from “electrons to reactors”. Design of materials for catalysis requires an understanding of catalyst structure, reaction pathways, and reactor characteristics that all must be combined to create a catalytic system. We have assembled a multidisciplinary team with expertise unique to ORNL to exploit existing knowledge and capabilities in multi-scale computational simulations, catalysis, materials characterization, and in situ spectroscopy to address these requirements. We will provide “proof of concept” and validation for our approach by comparing experimental data for a specific catalytic system to computational results at each length scale of the developed methodology. Specifically, we will generate an atomistic lattice model for reactive and diffusive surface catalytic processes for which kinetic data will be provided and averaged over the time domain. Coupling of the catalytic elementary steps with a reactive-transport model will permit understanding of macroscopic properties based on high-level atomistic predictions in a bottom-up approach. The result will be, for the first time, an atomic-to-macroscale description of catalysis over all the relevant spatial and temporal scales. Although we choose a specific catalytic system, our methodology is general, and it leads to a new capability for design of catalytic systems. This effort will establish ORNL as a leader in this area and prepare ORNL for a new call in computational materials sciences to develop community codes for the design of functional materials.

Research Project #2

**Title:** Application Data Structure Layout and Access Pattern Port Planning for Exascale Memory Architectures

**Principal Investigator:** Christos Kartsaklis, Computer Science Research Group, Computer Science and Mathematics Division, kartsaklisc@ornl.gov, 865-574-0159.

**Project Description:** The purpose of this project is to devise a memory-architecture centric co-design tool for determining how the data structures of parallel applications need to change in layout, redundancy, and distribution for future Exascale systems. This will allow reasoning about the performance/energy gains and associated software reengineering costs: to be able to
Research Project #3

Title: Predicting Climate Feedbacks from Microbial Function in Tropical Ecosystems

Principal Investigator: Melanie A. Mayes, Earth and Aquatic Sciences Group, Environmental Sciences Division, mayesma@ornl.gov, 865-574-7336.

Project Description: The soil microbial community exerts significant control over complex ecosystem function. The most ambitious theories suggest that functional traits of a community, e.g., methanogenesis and phosphate scavenging, can be used to predict environmental outcomes, e.g., soil nutrient availability and CO2 and CH4 emissions. In this pilot study, we will use metagenomics and other measurements to attribute functions to soil microbial communities along gradients of phosphorus availability and precipitation in Panama. We will manipulate moisture and phosphorus in the lab to effect changes in the metagenome, enzyme activities, and other indicators, thus enabling correlations between community functional profiles and climate feedbacks such as CO2 and CH4 emissions. We hypothesize that the balance of methanogens over methanotrophs will be significantly shifted in response to increased moisture, and that metagenomics can identify changes in the functional profiles of a soil community to facilitate predictive modeling of emissions. Adding P will further increase CO2 and CH4 emissions, particularly in P-limited versus P-rich soils. We will build correlations between community functional profiles and experimental observations of emissions designed to inform climate models. Our work will enable scaling of complex ecosystem functions from genes to functional groups to understand how organisms interact under natural environmental conditions and influence climate, and will position ORNL for leadership in BER's NGEE tropics.

Research Project #4

Title: Increasing Advanced Biofuels Production from Terpenes in Eucalyptus Leaves

Principal Investigator: Jerry Tuskan, Plant Systems Biology, Biosciences Division, tuskanga@ornl.gov, 865-576-8141

Project Description: Terpenes have the highest energy density and affordable conversion efficiency of any biofeedstock. Research proposed here focuses on maximizing production,
reducing volatilization and optimizing terpene content in Eucalyptus leaf oil glands (OG) for the creation of advanced fungible biofuel production in the U.S. By combining metabolic characterization, neutron scattering and transcript profiling, we will gain molecular-level insights into the determinant properties for synthesis and storage of terpenes in oil glands. Collectively, defining the genetic mechanisms of Eucalyptus leaf OG structure and chemistry will enable future applications of these resources for the genetic improvement of foliar OG number and volume, coupled with enhanced synthesis and storage of volatile and non-volatile terpenes. The scientific objectives are to select individual Eucalyptus genotypes that have high potential for terpene production and to identify the genes that control biochemical and anatomical features of favorable terpene production.

Research Project #5

Title: Theory of Neutron Scattering in Strongly Correlated and Disordered Materials

Principal Investigator: Thomas A. Maier, Computational Chemical and Materials Sciences Group, Computer Science and Mathematics Division, maierta@ornl.gov, 865-576-3597

Project Description: The ability to understand and predict the behavior of solids is key to accelerating the discovery of new materials and their rapid deployment into new technologies. The goal of this project is to develop a new theoretical capability to simulate magnetic neutron scattering experiments for a class of systems known as strongly correlated electron materials, which offer particularly exciting prospects for applications due to their complex emergent behavior and exotic physical properties. We have two immediate aims: (1) To formulate and implement a combined electronic structure and random phase approximation framework to enable simulations of a broad range of materials with strong disorder and weak to moderate correlations; and (2) to develop efficient and controlled procedures to extract dynamical quantities from complementary quantum Monte Carlo simulations of systems with strong correlations. The resulting suite of tools will allow us to perform quantitative and predictive simulations of a wide range of materials and to understand and predict the magnetic structure factor $S(Q, \omega)$. This quantity is directly measured in neutron scattering experiments at the SNS and elsewhere and thus provides an ideal observable to test and confirm or reject the hypothesis made with the simulations. As a proof of principle, we will use these tools to study iron- and copper-oxide based high-temperature superconductors, for which we have high hopes of unraveling one of the most important problems at the forefront of science, the nature of the pairing mechanism.
Research Project #6

Title: National Extreme Events Data and Research Center (NEED) – Transforming the National Capability for Resilience to Extreme Weather and Climate Events

Principal Investigator: Dale Kaiser, Environmental Sciences Division and Climate Change Science Institute, kaiserdp@ornl.gov, 865-241-4849

Project Description: The ORNL Climate Change Science Institute (CCSI) will develop and implement a novel concept to transform how the US studies and prepares for extreme weather events in the context of a changing climate – the National Extreme Events Data and Research Center. Our goal is to position ORNL as the home within DOE and the federal government for integrated scientific research and tool development for resiliency to climate- and weather-related extreme events, while supporting innovative basic and applied research on forecasting and adapting to such events. The project integrates two distinct components: (1) a new NEED database compiling global historical data on weather- and climate-related extreme events and related information about impacts, costs, recovery, and available research; and (2) a novel extreme weather events analysis and modeling approach that will leverage the NEED database and several other key weather and climate databases. We call this research “Monster Ridges” (MR) in reference to the strong upper-air ridges typically associated with extreme weather. We will bring meteorologists, data and computation experts, and climate modelers together to develop a novel application of machine learning (ML) to link ridging aloft to extreme events on the ground. Metrics and algorithms developed in our ML analysis will be used to probe a high-resolution-atmosphere climate model for its ability to simulate atmospheric dynamics that lead to extreme events, leading to improved predictions and model projections. We will focus on extreme heat events because they are relatively frequent and data are readily available and reliable. After solidifying our approach on heat events, we will extend the paradigm to other types of extremes, such as heavy precipitation (both rain and snow), violent storms, etc.

The HPC-related components of the project pertain to the MR research described above, specifically along three lines: (1) a machine learning approach to linking MR events with extreme surface temperature requires parallelizing GP for large spatiotemporal, (2) long simulations with high spatial resolution needed to capture sufficient events for the MR algorithm to generate robust statistics require large allocation of computer time on LCF, and (3) applying various MR/ML-derived metrics to climate model baseline data from several alternatively forced simulations for comparison to observational data and characterization of extreme, ridge-influenced events involves large data processing resources.
Research Project #7

**Title:** Functional Domains in Model Membranes and Protocells Probed with High-Performance Simulation and Neutron Scattering

**Principal Investigator:** Xiaolin Cheng, Center for Molecular Biophysics, Computer Science and Mathematics Division, chengx@ornl.gov, 865-576-0850.

**Project Description:** Cell membranes, once thought to be homogeneous assemblies of lipids and proteins, are now believed to contain nanoscopic domains (“lipid rafts”) critical to their function, particularly in transducing signals across the membrane. One persistent mystery in this regard is whether rafts bridge the two bilayer halves (leaflets), and how they could do so despite strong asymmetry in the composition, i.e., the presence of different lipids with distinct physical properties in the two bilayer leaflets. Resolving this mystery requires detailed structural information that has heretofore been unobtainable, because rafts are disordered and transient entities, and their size is below the detection limits of commonly-used biophysical characterization techniques. We propose technological development of high-performance computer simulation, model membrane platforms and neutron scattering experiments that will allow us to address this key outstanding question in membrane biology namely, how are lipid domains (rafts) on opposite sides of an asymmetric bilayer coupled? Neutron scattering will be used to study membrane vesicles that are, like natural cell membranes, compositionally asymmetric. Atomistic molecular dynamics simulations of the experimental system will be performed using ORNL’s TITAN supercomputer together with innovative and scalable sampling algorithms; the simulated system will comprise ~60 million atoms, and span time scales between 10 and 100 μs. The combination of leading edge experimental and computational techniques proposed here will provide new insights into the structure of biologically relevant membranes and their fundamental mechanisms underlying cell signaling and other biological processes.

Research Project #8

**Title:** Integrated Framework for Urban Climate Adaptation Tool (Urban-CAT)

**Principal Investigator:** Olufemi (Femi) Omitaomu, Geographic Information Science and Technology, Computational Sciences and Engineering Division, omitaomua@ornl.gov, 865-241-4310.

**Project Description:** Cities have an opportunity to become more resilient to climate change through changes made to urban infrastructure today. Comprehensive characterization of the
complex urban landscape and its critical infrastructure is newly possible as a result of recent advances in computing, simultaneous with the collection and integration of large disparate datasets. Higher resolution earth system models are now advancing to the point of being able to directly characterize future climate conditions at scales vitally needed by urban decision makers. The objective of this project is to develop a tool that will make America’s communities more resilient to climate change by helping urban governments: (1) understand climate change impacts on key infrastructure (e.g., water); (2) identify and prioritize adaption options (e.g., green infrastructure emplacement) for minimizing projected impacts; and (3) explore potential benefits of the adaptation options under different scenarios in relation to urban growth and infrastructure evolution. Integration of climate model outputs with infrastructure data will help local governments understand potential tradeoffs between urban planning objectives and (hidden) risks due to climate change and will help the climate modeling community to better understand the data and tools needed by urban decision makers. Therefore, there is a need for high resolution modeling (modeling at a neighborhood scale) of climate impacts on urban infrastructure using high performance computing capabilities. The outputs of such a model will be used as inputs into an integrated urban climate adaptation tool that will be developed.

Research Project #9

Title: An Integrated Approach to the Design and Discovery of Fast Ionic Conducting Materials

Principal Investigator: Panchapakesan Ganesh, Nanomaterials Theory Institute, Center for Nanophase Materials Sciences, ganeshp@ornl.gov, 865-574-1999.

Project Description: Our overarching goal is to discover by design, fast ionic conducting materials for energy storage and conversion technologies by integrating ORNL’s unique leadership in materials theory & computations, database management, materials synthesis and advanced characterization techniques. The focus on ionic transport is unique and timely because all the “Materials by design” efforts to-date have focused on thermodynamic stability with no concerted effort or rational approach to optimize ionic transport which fundamentally limits performance of virtually all energy materials. We propose an integrated approach to understand, predict, and demonstrate ways to optimize ionic conductivities by changing the migration barriers and the energetics of ion adsorption sites. This will be achieved identifying and controlling the local chemistry/structure via chemical substitution and/or strain (i.e., mechano-chemical coupling). We will use this approach to computationally optimize crystal structures that are known to exhibit proton/oxygen conductance by using high-throughput modeling, optimizing ionic conductivities at operating temperatures with the degree of alloying and also create a database & query system. Promising materials will be synthesized and
characterized using various methods including electron microscopy and neutron scattering. This data will be incorporated into the computational models improving their fidelity, building a powerful integrated “materials by design” transferable capability at ORNL to discover materials by design, which does not exist in competing institutions.

Research Project #10

**Title:** CloneX: Discrete Event Cloning at Exascale

**Principal Investigator:** Kalyan S. Perumalla, Discrete Computing Systems, Computational Sciences and Engineering Division, perumallaks@ornl.gov, 865-241-1315.

**Project Description:** To overcome the challenges with respect to concurrency and memory in achieving Exascale computing, we are designing, developing, and implementing a novel technique of large-scale, transparent, and optimized "cloning". The project develops the conceptual framework, the algorithmic foundations, and a prototype interface with implementation of runtime system scaling to hundreds of thousands of processor cores, and tests the new technology with example applications whose aggregate concurrency and memory needs are increased from petascale by orders of magnitude. The research will (a) demonstrate a novel way to exploit Exascale computing capability for a wide range of applications that fall short in scaling potential to Exascale in the traditional sense, (b) show orders of magnitude reduction in aggregate memory requirement, (c) demonstrate a naturally effective fault tolerant mode, and (d) deliver an optimized and scalable cloning runtime system suitable for multiple applications.

Research Project #11

**Title:** Fine-resolution Modeling of Urban-Energy Systems’ Water Footprint in River Networks

**Principal Investigator:** Ryan A. McManamay, Energy-Water Resource Systems Group, Environmental Sciences Division, mcmanamayra@ornl.gov, 865-241-8668.

**Project Description:** Characterizing the interplay between urbanization, energy production, and water resources is essential for ensuring sustainable population growth. Water is a critical resource, supporting infrastructure, societal needs, and ecosystem services upon which humans depend. In order to balance limited water supplies, competing users must account for their realized and virtual water footprint, i.e. the total direct and indirect net amount of water consumed, respectively. Unfortunately, publicly reported US water use estimates are spatially
coarse, temporally static, and completely ignore returns of water to rivers after use. These estimates are insufficient to account for water budgets in urbanizing systems characterized by high spatial and temporal heterogeneity in infrastructure, population demographics, and subsequent water use. Likewise, urbanizing areas are supported by competing sources of energy production, which also have heterogeneous water footprints. Hence, a fundamental challenge of planning for sustainable urban growth (and decision-making across disparate policy sectors) lies in characterizing inter-dependencies among urban systems, energy producers, and water resources. A modeling framework is presented at an unprecedented scale that provides a novel approach to integrate urban-energy infrastructure into a spatial accounting network that accurately measures water footprints as changes in the quantity and quality of river flows. River networks (RNs), i.e. networks of branching tributaries nested within larger rivers, provide a spatial structure to measure water budgets by modeling hydrology and accounting for use and returns from urbanizing areas and energy producers. The research team proposes the following objectives: 1) develop a dynamic RN modeling framework that accounts for water budgets from the urban-energy interface as changes to river systems, 2) characterize the current and future water footprints of integrated urban-energy systems, and 3) examine tradeoffs among urban-energy development, water resources, and natural river ecosystem sustainability.

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**Research Project #12**

**Title:** *Algorithms for Context-Specific Analysis of Heterogeneous Unstructured Big Health Data*

**Principal Investigator:** Georgia Tourassi, Biomedical Sciences and Engineering Center, Computational Sciences and Engineering Division, tourassig@ornl.gov, 865-576-4829.

**Project Description:** High-dimensional, multi-modal, unstructured data poses significant visual and computational analytic challenges. Data-driven knowledge discovery is severely crippled when domain experts tend to limit their attention to data subsets because they are overwhelmed with data volume and complexity. For example, in medicine mining heterogeneous data such as patients’ genome sequences, images, and sensor data in context with prior history for clinical decision support is an outstanding problem. The complexity of the problem is not just data volume (e.g. genome sequences are several gigabytes/person, image databases in the order of terabytes, etc.) but data variety. To address the emerging problems where data variety trumps volume, we are proposing: (1) a data organizing framework to discover and store associations across trans-disciplinary unstructured datasets; (2) scalable in-memory methods for multi-modality similarity discovery; and (3) an informative, context-adaptive display to explore, prioritize, and visualize recommendations of relevant associations.
that would have otherwise overwhelmed the human perceptual and cognitive bandwidths. This framework will show proof-of-principle for health data, enabling an order increase improvement in processing time and informative visualization while integrating and analyzing multi-modal, complex health data. The underlying scientific principles for data organization, association, and knowledge discovery will extend to other application domains beyond medicine.

Research Project #13

Title: Interrogating Monolignol Transport Using a Multimodal Imaging Approach

Principal Investigator: Jennifer Morrell-Falvey, Biological and Nanoscale Systems, Biosciences Division, morrelljl1@ornl.gov, 865-241-2841.

Project Description: Lignin is the second most abundant biopolymer on earth. Mechanically robust and structurally complex, lignin is important for maintaining the structural integrity of the plant cell wall. However, lignin is seen as a major contributor to the wall’s recalcitrance to hydrolysis, and is viewed as problematic in the paper and biofuels industries. Conversely, there is growing appreciation for the potential of lignin in the production of engineered materials and specialty chemicals. Whether the goal is to minimize the recalcitrance of biomass or to engineer new products, a deeper understanding of lignin biology is needed to enable manipulation of lignin content and composition in the cell wall for downstream applications. Lignification of plant walls can be described in three steps: biosynthesis of monolignols in the cytoplasm, transport of the monolignols across the plasma membrane, and polymerization of monolignols into the cell wall. Although there has been much research on monolignol biosynthesis, there is surprisingly little known about the transport of these monolignols across the plasma membrane. Recently, a breakthrough in our understanding of monolignol transport came with the identification of an ATP-binding cassette (ABC) transporter in Arabidopsis thaliana that specifically transports p-coumaryl alcohol [Curr. Biol 2012 22(13):1207]. We hypothesize that the variation of lignin content and composition in different tissues and cell types is due, in part, to spatial and temporal expression of the monolignol transporters. Our experimental approach will involve generation of a tagged monolignol transporter protein and synthesis of tagged monolignol analogs that will enable interrogation of the same sample with multiple imaging methods, including high resolution fluorescence microscopy, transient absorption microscopy and electron microscopy. At present, correlated imaging measurements are difficult to achieve because each imaging method is specialized and requires specific sample preparation or imaging probes that may not be compatible with other imaging platforms. Overcoming this obstacle requires a deliberate effort to coordinate biologists, chemists and analytical scientists
to design and construct multi-purpose probes and samples that can be shared between imaging platforms. The use of multiple imaging methods will strengthen the scientific impact of these studies by adding complementary information and overcoming limitations associated with individual imaging methods.

Research Project #14

Title: *Optimizing HFIR Isotope Production through the Development of a Sensitivity-Informed Target Design Process using High-Fidelity Modeling and Simulation Capabilities*

Principal Investigator: Bradley T. Rearden, Reactor and Nuclear Systems Division, reardenb@ornl.gov, 865-574-6085.

Project Description: The goal of this project is optimizing isotope production in the ORNL High Flux Isotope Reactor (HFIR) through the investigation and demonstration of recent breakthroughs in sensitivity and uncertainty analysis on high-performance computing (HPC) platforms. Specific aims of this work include: 1) investigation of state-of-the-art sensitivity and uncertainty analysis algorithms for use in ORNL HPC modeling and simulation (M&S) tools, (2) development of a prototypic isotope production optimization technique using sensitivity analysis to guide enhancements in HFIR target and filter design parameters, and (3) better informing HFIR facility safety assessments by quantifying the sources and impact of uncertainty in design-limiting irradiation target heat generation calculations. Completion of these tasks will enable scientists to utilize a sensitivity-informed irradiation target design process in future campaigns, and the success of this work will position ORNL with a unique capability for performing state-of-the-art sensitivity analysis using cutting-edge HPC tools.

Research Project #15

Title: *Integrated Energy Systems*

Principal Investigator: Roderick Jackson, Building Technologies Research and Integration Center, Energy and Transportation Science Division, jacksonrk@ornl.gov, 865-241-8809.

Project Description: There are three primary physical systems that must be integrated to achieve an effective and resilient off-grid building (OGB): energy generation, energy storage, and building energy demand. In addition to the need for high performing systems, to achieve cost competitiveness, ensure required performance criteria, and maintain system constraints, these components must be optimally integrated and dynamically managed. The optimal
solution must consider uncertainty while trying to find a solution that meets the occupant’s demand on an hourly, daily, monthly and yearly basis. To meet this challenge, the proposed project utilizes a fully integrated approach to address the off-grid building challenge in three distinct manners: (1) develop advanced generation and storage systems to provide a demonstration for new technologies that can enable cost effective off grid buildings; (2) develop an off-grid building management system (OBMS) to optimally integrate and manage the building load, distributed generation, and required energy storage; and (3) utilize a use-inspired approach to understand the science needed to make transformative breakthroughs in energy storage.

Research Project #16

Title:  High Resolution Solid State Neutron Detectors for Second Target Station

Principal Investigator:  Richard A. Riedel, Instrument Projects and Development, Instrument and Source Division, riedelra@ornl.gov, 865-576-2674.

Project Description:  This project focuses on Li containing ZnSe and ZnO based chalcogenides as potential high light yield neutron sensitive scintillators. Theory based on first principles calculations will be used to obtain the electronic structures and to predict scintillation and optical properties. The calculations will allow quantitative prediction of band gaps, band gap type (direct vs. indirect) and matching of valence and conduction band masses, which are important in determining the likelihood that a material can be developed into an efficient low temperature scintillator. Theoretical results will be used in selecting compounds most suited to experimental investigation, helping guide optimization of the materials and in interpreting experimental results. Feedback from characterization of the synthesized crystals will provide an avenue to improve the predictive power of the first principles calculations.

Research Project #17

Title:  Scalable Data and Informatics for Connected Vehicles Leveraged to Enhance Efficiency

Principal Investigator:  Andreas Malikopoulos, Deputy Director, Urban Dynamics Institute, Energy and Transportation Science Division, andreas@ornl.gov, 865-946-1529.

Project Description:  Recognition of the necessity for connecting vehicles to their surroundings is gaining momentum. Many stakeholders intuitively see the benefits of multi-scale vehicle control systems and have started to develop business cases for their respective domains,
including the automotive and insurance industries, government, and service providers. The main focus is on safety and how accidents could potentially be prevented by alerting drivers. The question is whether we could take advantage of connected vehicle technologies and optimize efficiency of the vehicles in addition to safety. This project will directly address the appropriate conceptual approaches for modeling and optimization aimed at coordinating a fleet of connected vehicles to improve efficiency. The long-term potential benefits of the proposed research are substantial. Overall operation of vehicles can be improved in terms of fuel economy and GHG emissions. Coordination of vehicles through instructions provided to drivers will help avoiding congestions, and thus eliminating stop-and-go driving and idle engine operation enabling additional fuel savings and improving comfort.

Research Project #18

Title: Spatially Resolving Electron Spin Dynamics and Transport in Low-Dimensional Materials

Principal Investigator: An-Ping Li, Center for Nanophase Materials Sciences, apli@ornl.gov, 865-576-6502.

Project Description: Low-dimensional materials are predicted to have intriguing properties associated with electron spin, e.g. interfacial magnetism in oxides, half-metallicity at graphene edges, and topologically protected skyrmion states in chiral magnets, many of which have remained elusive to validation. One way to understand the role of electron spin is to combine information on an atomically precise geometry with the local spin-dependent electronic density of states, and correlate them with charge and spin transport over different length scales. Spin-polarized scanning tunneling microscopy (SP-STM) represents significant progress towards this goal; the approach however is limited to probing static charge and spin densities. Spatially resolving spin dynamics and transport is still not possible through SP-STM. We propose a spin-polarized scanning tunneling potentiometry (SP-STP) approach to resolve spin dynamics and transport. SP-STP simultaneously records real-space information on geometry, electronic structure, spin, and electrochemical potentials that drive charge and spin currents in a mesoscopic system. The effort is guided and complemented by first-principles and analytical calculations. The goals are (1) establishing a spin-dependent multi-scale spectroscopy approach, which provides an accurate description of electronic behavior associated with the spin degrees of freedom, such as spin-dependent conductivity, spin diffusion length, and spin injection efficiency, and (2) applying this approach to outstanding properties of low-dimensional materials dictated by defects, boundaries, and interfaces.