Title: Performance Analysis, Modeling and Scaling of HPC Applications and Tools

Principal Investigator: Abhinav Bhatele, *Lawrence Livermore National Laboratory*

Co-Investigators: Laura Carrington (*SDSC*), Todd Gamblin (*LLNL*), Jeffrey K. Hollingsworth (*U. Maryland*), Laxmikant V. Kale (*U. Illinois*), Steven H. Langer (*LLNL*), Allen D. Malony (*U. Oregon*), Martin Schulz (*LLNL*), Sameer Shende (*U. Oregon*), Nathan R. Tallent (*PNNL*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	20,100,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	9,300,000 processor hours

Research Summary

Efficient use of supercomputers at Department of Energy centers is vital for maximizing system throughput, minimizing energy costs and enabling science breakthroughs faster. This requires complimentary efforts along several directions to optimize the performance of scientific simulation codes and the underlying runtimes and software stacks. This in turn requires providing scalable performance analysis tools and modeling techniques that can provide feedback to physicists and computer scientists developing the simulation codes and runtimes respectively.

This project supports time allocations on supercomputers at Argonne Leadership Computing Facility (ALCF, Argonne National Laboratory) and Oak Ridge Leadership Computing Facility (OLCF, Oak Ridge National Laboratory) to further the goals described above by performing research along the following fronts: 1. Scaling Study of HPC applications; 2. Evaluation of Programming Models; 3. Hardening of Performance Tools; 4. Performance Modeling of Irregular Codes; and 5. Statistical Analysis of Historical Performance Data. This project will enable investigations into big data issues when analyzing performance data on leadership class computing systems and to assist the High Performance Computing (HPC) community in making the most effective use of these resources.

The allocation time supports research and development of computer science efforts in the areas of computational science applications, programming models, runtimes, and performance tools and models that will help prepare the HPC community for exascale.

Title: Introducing Carriers and Control Polaronic States in Energy-related Complex Solids

Principal Investigator: Alex Zunger, *University of Colorado at Boulder*

Co-Investigators: Y. G. Yu (*UC Boulder*), X. Zhang (*UC Boulder*), Q. Liu (*UC Boulder*), G. Trimarchi (*Northwestern U*)

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 10,000,000 processor hours

Research Summary

Most energy relevant technologies are based on materials with specialized properties, which tend to exist in specific materials, and no others. For transport-based devices, one needs stable, low cost materials having superior electronic transport properties needed in photovoltaics, photocatalysis, flat panel and touch screen technology. Finding materials with these special properties is a leading challenge in establishing efficient energy technologies.

This project supports research to identify, out of a huge number of possibilities, which materials have the specific properties needed for transport based energy technologies. This project combines advanced Quantum Theory of Matter with fast and efficient supercomputers to screen a large material space. Specifically, this project will screen for the ability of the material (a) to 'allow' injection of free electrons and holes into it, and (b) permit such charges to freely move through the solid. Interestingly, very few materials have these properties, and testing all of these in the laboratory one at the time is not a tenable proposition. Yet, such materials would unlock efficient solar cells, touch screen and flat panel displays and fast transistors. This research team has developed a computational 'Litmus Test' that would identify the compounds most likely to qualify the stringent requirement, and thus enable experimentalists to focus just on the most promising candidates.

Title: Dynamics of Magnetic Fields in High-Energy-Density Plasmas from Fusion to Astrophysics

Principal Investigator: Amitava Bhattacharjee, *Princeton Plasma Physics Laboratory*

Co-Investigators: Kai Germaschewski (*UNH*), William Fox (*PPPL*), Yi-Min Huang (*Princeton U.*), Jonathan Ng (Princeton U.)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 45,000,000 processor hours

Research Summary

Plasma, like solids, liquids and gas, is a state of matter. In solids, liquids and gas, atoms hold onto electrons through interactions between the nucleus and the electron. In plasma, however, the atoms have been stripped of their negatively charged electrons and exist as positively charged atoms, or ions. In plasma, the ions and electrons interact and display a rich spectrum of collective effects but are not bound together. Plasma is not as readily apparent in everyday life as the other states of matter, yet plasma science has special importance for our planet and life. Plasma is the primary form of matter in the Sun and is also a key ingredient to a potential limitless supply of green-energy for the world, fusion energy. In both cases, the interaction between plasma and magnetic fields is key to understanding some of the most important aspects of plasma physics in both the laboratory and in outer space. While in magnetic fusion, the interaction between plasmas and the external as well as internally generated magnetic fields is an essential component of the confinement method, in inertial fusion, understanding the role of magnetic fields is a relatively new development. Due the importance of the interaction between plasmas and magnetic fields in the context of inertial fusion as well as astrophysical plasma physics, there have been recent investments in new high-energy-density physics facilities and laboratories, including both laser facilities and pulsed power systems. These facilities have opened significant physics opportunities both for fusion and for experimentally modeling astrophysical plasmas.

This project supports investigations to understand and model the dynamics of magnetic fields in these high-energy density plasmas, including their generation, subsequent dynamics, and annihilation. These involve processes such as magnetic field generation followed by reconnection that liberates stored magnetic energy in phenomena as diverse as 'sawtooth crashes' in fusion plasmas, magnetospheric substorms, and solar flares. This project directly connects simulation and experiment, through collaboration with researchers at the Laboratory for Laser Energetics at the University of Rochester. From astrophysics to the possibility of a controlled sustained fusion reactor, results of this project will increase our fundamental understanding of high-energy density plasmas and their interactions with magnetic fields.

Title: Credible Predictive Simulation Capabilities for Advanced Clean Energy Technology Development through Uncertainty Quantification

Principal Investigator: Aytekin Gel, *ALPEMI Consulting, L.L.C. /NETL*

Co-Investigators: Mehrdad Shahnam (*NETL*), Arun Subramaniyan (*GE Global Research Center*), Jordan Musser (*NETL*), Jean-François Dietiker (*WV University Research Corporation /NETL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory

Allocation: 111,500,000 processor hours

Research Summary

Advanced power generation processes such as the Integrated Gasification Combined Cycle (IGCC) offer the promise of allowing continued use of coal as a power source while reducing carbon dioxide emissions. The IGCC converts coal into synthesis gas (syngas), and then cleanly burns the hydrogen in the syngas. Integrating all of these processes into a single combined cycle allows efficient energy production, while allowing carbon dioxide to be captured for storage. However, the cost of design and scale-up testing for commercial scale IGCC remains a barrier to using this technology.

Advanced modeling and simulation capabilities, which may reduce or even avoid prototype testing, is one route to reducing these costs. However, this requires that the simulations be trusted by the design community. Research is being carried out at the National Energy Technology Laboratory (NETL), to establish credibility in simulation results from a fluidized bed gasifier by applying uncertainty quantification methods. Input uncertainty propagation through the Computational Fluid Dynamics (CFD) model has been employed in addition to Bayesian uncertainty quantification methods to quantify model discrepancy in the simulation results. A comprehensive assessment of predictive simulation capabilities is sought by identifying and quantifying various sources of uncertainties. A credible predictive capability based on these computational models is crucial in scale-up studies as a decision support tool in reducing time-to-market deployment of advanced clean coal energy technologies.

Title: Cloud-System Simulations with a Multiscale Nonhydrostatic Global Atmospheric Model

Principal Investigator: William D. Collins, *Lawrence Berkeley National Laboratory*

Co-Investigators: James J. Benedict (*LBNL*), Elijah Goodfriend (*LBNL*), Hans Johansen (*LBNL*), Jeffrey Johnson (*LBNL*), Noel D. Keen (*LBNL*), Travis A. O'Brien (*LBNL*), Daniele Rosa (*LBNL*)

ALCC allocation: Processor Hours

Site: Lawrence Berkeley National Laboratory

Allocation: 56,000,000 processor hours

Research Summary

Many atmospheric phenomena with the greatest potential impact in future warmer climates are inherently multiscale. Such meteorological systems include hurricanes and tropical cyclones, atmospheric rivers, and other types of hydrometeorological extremes. These extremes are challenging to simulate in conventional climate models due to the models' relatively coarse resolutions relative to the native length-scales of these phenomena.

To enable studies of these systems with sufficient local resolution yet with sufficient speed for climate-change studies, we have developed an atmospheric model with adjustable spatial resolution. The dynamics is based upon an adaptive, conservative finite volume approach suitable for moist non-hydrostatic atmospheric dynamics. By using both space- and time-adaptive mesh refinement, the solver allocates computational effort only where greater accuracy is needed to resolve critical phenomena. The resulting model is designed and proven to be both highly accurate and highly scalable for massively parallel supercomputers. We have combined these dynamics with the physics used in superparameterized versions of DOE's Accelerated Climate Model for Energy (ACME). In superparameterization, conventional statistical representations of clouds and convection are replaced with explicit dynamical representations for greater fidelity to observed atmospheric processes.

This ALCC allocation supports testing of this new model at cloud-resolving scales and to evaluate its suitability for examining changes in clouds and convection in a warmer climate. If successful, this model would represent the first successful prototype of a global atmospheric model with adaptive mesh resolution. It would also represent DOE's first non-hydrostatic cloud-resolving atmospheric model suitable for future exascale computers.

Title: Understanding Helium-Hydrogen Plasma Mediated Tungsten Surface Response to Predict Fusion Plasma Facing Component Performance in ITER

Principal Investigator: Brian Wirth, *University of Tennessee*

Co-Investigators: Blas Uberuaga (*LANL*), Karl Hammond (*U. Missouri*), Rick Kurtz (*PNNL*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	80,000,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	36,000,000 processor hours

Research Summary

The realization of fusion as a practical, 21st Century energy source requires improved knowledge of material surfaces and their interaction with the fusion material. In current fusion reactor designs, fusion energy is created from the fusion of hydrogen into helium atoms. In a reactor, fusion occurs in an extremely hot helium-hydrogen plasma that necessarily interacts with the material of the containment vessel. For successful design of a fusion reactor the interaction of this hot plasma on the containment material must be understood for successful materials engineering design.

This allocation supports simulations to advance understanding of the response of tungsten, the proposed material for the ITER (an under-construction fusion reactor) divertor, to low energy helium and hydrogen plasma exposure. Knowledge of these interactions is necessary to identify materials design strategies to effectively manage high gas exposures expected in the fusion energy environment, and to quantify the expected inventory of radioactive tritium stored within the plasma facing components. This project will perform simulations at both the atomistic and continuum scale for comparison and benchmarking, as well as the identification of appropriate reduced-parameter models to describe complex, multiscale phenomena controlling gas behavior in fusion materials. The outcome will be a greater physical understanding and predictive modeling capability for materials design of the divertor for ITER.

Title: Three-dimensional Simulations of Core-collapse Supernovae from High-mass Progenitor Stars

Principal Investigator: Bronson Messer, *Oak Ridge National Laboratory*

Co-Investigators: J.M Blondin (*NCSU*), S.W. Bruenn (*FAU*), E.J. Lentz (*UTK*), W. R. Hix (*ORNL*), A. Mezzacappa (*UTK*), K. Yakunin (*UTK*)

ALCC allocation: Processor Hours

Site: Oak Ridge National Laboratory

Allocation: 48,000,000 processor hours

Research Summary

Core-collapse supernovae mark the death of massive stars and the birth of neutron stars and black holes. The 3D supernova simulations proposed here will explore the fate of the largest massive stars we believe experience these gigantic explosions – stars up to 25-30 times the mass of our own sun. The simulations will be performed using the Chimera multiphysics supernova code. Chimera contains all of the relevant physics required for core-collapse supernova simulations including transport of energy by neutrinos and the required neutrino-matter interactions, general relativity and self-gravity, nuclear burning and nuclear equations of state, and 3D fluid dynamics. The core-collapse supernova problem has been a computational challenge for several decades, but now we have entered an era in which well resolved, symmetry-free 3D simulations are now possible. From the simulations the project will examine the differences between the core-collapse supernova mechanism in these 3D simulations and in 2D (axisymmetric) simulations. Researchers will also generate neutrino and gravitational wave signals that could be expected in detectors here on Earth from a nearby supernova, which directly probe the explosion mechanism. By including detailed nuclear reactions in the simulations, the simulations will generate detailed isotopic and elemental compositions of the material ejected by the supernova, which recent studies suggest will be quite different from current nucleosynthesis models that ignore the neutrino-driven, multidimensional nature of the explosion. These simulations will also be used to calibrate and correct larger sets of simpler models that are used to examine the detailed diversity of presupernova massive stars. Outcomes of this project will advance our understanding of nuclear physics and the processes involved in the universes largest explosions.

Title: Simulating Multiphase Heat Transfer in a Novel Receiver for Concentrating Solar Power (CSP) Plants

Principal Investigator: Christina Hrenya, *University of Colorado*

Co-Investigators: Aaron Morris (*U. Colorado*), Sreekanth Pannala (*ORNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 5,000,000 processor hours

Research Summary

Efficient, large scale, and cost effective mechanisms for harvesting energy from the sun would have profound impacts on the clean energy sector and reductions in the use of fossil fuel. Concentrated Solar Power (CSP) is a promising technology which collects heat energy from the sun by reflecting sunlight (via mirrors) from a large surface area onto a much smaller area. The reflected sunlight heats a receiver substance which then travels to a power station where the heat is used to drive a turbine that creates electricity. The success of the CSP technology relies heavily on the heat absorption, storage, and transfer properties of the receiver substance in the CSP. However, there is a well-documented lack of reliability of empirical correlations for related systems and a fundamental model is necessary for purposes of design, scale-up, and optimization. This project supports multiphase flow and radiative heat transfer modeling of a potential receiver substance. Outcomes of this project will include state of the art codes that aid advances in CSP receiver substance design, and represent important steps towards clean energy.

Title: Chombo-Crunch: Modeling Pore Scale Reactive Transport Processes Associated with Carbon Sequestration

Principal Investigator: David Trebotich, *Lawrence Berkeley National Laboratory*

Co-Investigators: Brian Van Straalen (*LBNL*), Greg Miller (*LBNL*), Carl Steefel (*LBNL*), Sergi Molins (*LBNL*)

ALCC allocation: Processor Hours

Site: Lawrence Berkeley National Laboratory

Allocation: 50,000,000 processor hours

Research Summary

Carbon dioxide , CO2, is a well-known green-house gas emitted in many energy production and use technologies. A primary example is in coal burning electrical power generation. One method to prevent emittance of CO2 into Earth's atmosphere is to recapture the CO2 as it is emitted from an electric-generation plant and strategically sequester the CO2 underground. Many scientific and engineering questions must be answered before this method of carbon capture and sequestration can become a large-scale effective strategy against green-house gas emission.

This project supports research to answer key questions on CO2 geologic sequestration. Researchers will use direct numerical simulation at unprecedented scale and resolution to model pore scale processes associated with carbon sequestration and to bring such knowledge to bear on the macroscopic scale of a reservoir. Outcomes will support the objectives of the DOE Energy Frontier Research Center for Nanoscale Control of Geologic CO2 and help advance scientific understanding of an important mitigation technology.

Title: Toward a Longer-Life Core: Thermal-hydraulic CFD Simulations of Deformed fuel assemblies

Principal Investigator: Elia Merzari, *Argonne National Laboratory*

Co-Investigators: Paul Fischer (*ANL*), Aleksandr Obabko (*ANL*), Nate Salpeter (*Terrapower*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 72,000,000 processor hours

Research Summary
Nuclear energy provides a cost-effective carbon-free energy source. Advancing nuclear reactor technology is important for improving safety, lifetime duration, and reactor efficiency. Reactor's today use water as the primary cooling (and heat transfer source) for nuclear reactors. The development of liquid---metal---cooled fast reactors is a promising new reactor technology and has received increased interest in recent years with a particular focus toward longer life cores that maximize utilization of the nuclear fuel and plant availability.

In this project, TerraPower and ANL partner to study the effect of longer life core on the heat transfer and flow physics of SFR (Sodium Cooled Fast Reactor) nuclear assemblies, which are parts of the nuclear reactor core. In fact, long life cores present serious challenges: when assemblies age they are also increasingly damaged. The prediction of thermal performance in SFR fuel assemblies is of vital importance to evaluate overall reactor performance and the safety margins and thus to make a viable carbon---free energy production technology. This proposal is integral part of a well---defined validation program for the Thermal/Hydraulic Computational Fluid Dynamics (CFD) modeling of SFR, funded by DOE Nuclear Energy. Outcomes of this project will advance nuclear reactor technology and support the clean and safe energy agenda.

Title: High-fidelity Computations of Fuel Assemblies Subjected to Seismic Loads

Principal Investigator: Elias Balaras, *George Washington University*

Co-Investigators: Philippe Bardet (*GWU*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 34,000,000 processor hours

Research Summary

Pressurized Water Reactor (PWR) cores are especially sensitive to seismic events. The lateral displacements of the reactor core under seismic loads produce large lateral deformations, and as a result, the fuel rods can bend creating contacts between cladding and fuel pellets, and local hot spots. This may also prevent control rod insertion, which compromises safe reactor shutdown. Today, the safety analysis and design tools for core seismic loads are primarily based on empirical correlations and do not incorporate detailed physics of fluid-structure interaction problem due to the lack of detailed experiments and high-fidelity simulations. Although earthquake effects in PWR cores have been studied, available data are limited to rod vibration frequencies and local impact forces. More detailed information on the dynamics of the velocity and pressure fields has only been obtained for static conditions. Recent advances in mathematical models and algorithms enabled by the availability of high-end compute platforms with hundreds of thousands of cores, bring high-fidelity computations of these complex fluid structure interaction problems, within range. In the proposed computations the interaction of the flow with the fuel rods under extreme seismic loads will be simulated with an unprecedented level of detail. Our main objective is to illuminate the physics of this complex problem and provide the necessary data to develop calibrated semi-empirical models typically used in the design and safety analysis.

Title: Computational Design of Novel Multiscale Concrete Rheometers

Principal Investigator: George William, *NIST- National Institute of Standards and Technology*

Co-Investigators: Nicos S Martys (*NIST*), Judith Devaney Terrill (*NIST*), Marc Olano (*NIST*), Pascal Hébraud (*Institute of Physics and Chemistry (France)*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 50,000,000 processor hours

Research Summary
The science of rheology is concerned with the flow and deformation of materials under applied forces. Accurately measuring the rheological properties of complex suspensions like concrete is crucial and a widespread problem in the construction and other industries. Although rheology is important to the development, analysis, and optimization of cement based materials, its rheological properties cannot currently be measured accurately in industrial settings. Design and development of accurate rheometers, devices that measure rheological properties, could significantly advance the development of new products that are energy efficient to produce.

This allocation supports computer simulations of many thousands of particles, with a wide range of sizes and shapes and suspended in a cement paste, to enable the design of accurate rheometers that will advance the use of these instruments. The knowledge gained from these simulations will also enable the development of better and more energy efficient materials by reducing the time and cost required for such research and development efforts.

Title: Large-Eddy Simulation of Turbine Internal Cooling Passages

Principal Investigator: Gustavo Ledezma, *General Electric*

Co-Investigators: Sourabh Apte, Oregon State University

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 6,000,000 processor hours

Research Summary

The efficiency of gas turbine engines is determined by combustion temperature: hotter combustion temperatures lead to more efficient operation. However, higher combustion temperatures require active cooling to avoid melting individual turbine components. One method for doing this is serpentine channels through the turbine blades. These channels route air from the compressor through the interior of the turbine blades to cool the turbine blade, preventing the surface from melting. Understanding air flow through these channels is critical to making the cooling as efficient as possible, as well as predicting the reliability of the turbine.

This project will used advanced computational fluid dynamics to simulate the turbulent flow and heat transfer through the serpentine cooling passages of a system that has been well-studied experimentally: the Stanford University Canonical Turbine Cooling Case. Researchers will use Large-Eddy Simulation (LES) methods to accurately include the effect of turbulent flow in the passage. This will allow investigators to determine how recirculation zones, turbulent intensities, heat transfer coefficients, coolant pressure drops and particle transport characteristics change as the flow conditions change. Initial simulations will be performed on non-rotating cases, allowing researchers to validate their results with direct comparison to experimental data. The researchers will then move to simulation rotating cases, to match actual turbine conditions. Including the transport of small particles, such as dust or dirt swept into the engine, will improve predictions of erosion in these channels. Because even small gains in efficiency over the number of gas turbines in operation yield large gains in fuel economy over an entire fleet of turbines, the results of this study have the potential to lead to large improvements in energy efficiency.

Title: PT-symmetric Quantum Mechanics for Real-time Electron Transport Simulations

Principal Investigator: Hanning Chen, *George Washington University*

Co-Investigators: Wei Jiang (*Argonne National Laboratory*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 16,000,000 processor hours

Research Summary

The electronics-led information revolution has transformed nearly every aspect of human life. The transformative revolution was mainly triggered in the 1950s by the rise of semiconductor technology. Compute power per unit area (transistors per unit area) has grown exponentially according to Moore's Law, enabling modern micro-electronics and powerful embedded processors unthinkable only 50 years earlier. However, technology is pushing the physical limits of how small modern silicon devices can be fabricated. Molecular electronics is a promising solution to extend Moore's law beyond the quantum limit of silicon-based semiconductors. Despite the rapid progress of molecular electronics on the experimental side, the theoretical modeling of electron transport across nanoscale molecular devices remains a challenging task. The difficulty primarily lies in the fact that electron transport is intrinsically a non-equilibrium process in open systems while most well established theories were derived for closed systems in the adiabatic limit. In the proposed study, we plan to apply our newly developed time-dependent PT-symmetric approach featuring asymmetric transmission resonance potentials on some well-studied model transport systems for rigorous justification.
This project supports integrating the PT-symmetric quantum transport approach and the real-time time-dependent density functional theory into a massively parallel molecular simulation package. Once the project is accomplished, a solid theoretical and computational framework will be established for the systematic design of molecular electronics with desired electrical property.

Title: Predictive Modeling of Functional Nanoporous Materials

Principal Investigator: J. Ilja Siepmann, *University of Minnesota*

Co-Investigators: Michael W. Deem (*Rice U.*), Laura Gagliardi (*U. Minnesota*), Christopher Knight (*ANL*), David S. Sholl (*Georgia Tech*), Randall Q. Snurr (*Northwestern University*), Donald G. Truhlar (*U. Minnesota*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 120,000,000 processor hours

Research Summary

Nanoporous materials are crystalline or armorphous materials with a significant amount of void space in the form of channels and pores. Those with pore dimensions of 0.2–2 nm form the category of microporous materials, and those with pore dimensions of 2–50 nm are classified as mesoporous materials. Nanoporous materials are important to many industries and applications because the small dimensions/features of the porous material allow the material to interact on atomic and molecular scales and, hence, impart selectivity. Application areas include diverse sectors such as ion-exchange for water purification, or catalytic surface for chemical energy production. Designing diverse nanoporous materials to optimize their performance would be a large step forward for the chemical, oil & gas, and biotechnology industries.

This allocation supports an interdisciplinary team developing methods to accelerate the discovery and design of nanoporous materials with tailored functions for a variety of energy-related applications. Specific applications include nanoporous materials for upgrading of gasoline through the separation of hexane isomers with higher octane number from other isomers, for second-generation biofuel production by separation of butanol from fermentation broths, for purification of renewable feedstock compounds for high-value polymers, for methane storage with high deliverable capacity, for purification of unsaturated light hydrocarbons for olefin polymers, and for capture of carbon dioxide from flue gases. In addition, this research will contribute to the development of a computational infrastructure for screening and design of new heterogeneous catalysts and associated scaffolds. The outcome of this project will support new design methods for improved discovery and design of nanoporous materials.

Title: Exploring Quantum Optimizers via Classical Supercomputing

Principal Investigator: Itay Hen, *University of Southern California*

Co-Investigators: Daniel Lidar (*USC*), Tameem Albash (*USC*), Travis S. Humble (*ORNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 20,000,000 processor hours

Research Summary
Classical computers, that manipulate and store bits to perform calculations, have become incredibly powerful. Modern classical supercomputers can perform thousands of trillions of calculations in a single second. Yet many everyday problems will forever remain beyond the grasp of classical computers due to the vast time, often longer than the age of the universe, that would be needed to solve the problem. An important example is optimization problems. In certain optimization problems, scientists want to find the optimal solution from a vast space of options, for example 'what is the most energy efficient design for my engine'. Finding the true global solution to optimization problems is often classically hard (at times virtually impossible). Quantum computers offer a promising alternative to classical computers and may hold the key to efficiently solving hard optimization problems. Quantum annealing is an optimization technique for classically hard optimization problems. The quantum mechanism that could allow the advantage in quantum annealing is *quantum tunneling*, which under certain conditions allows the penetration of energy barriers by passing through classically-forbidden regions. As such, Quantum Annealers promise to solve optimization problems of great practical importance in many areas of Science, Government and Industry, faster than is possible on any classical computer.

Despite having been studied both theoretically and experimentally, to date there are no known physically relevant examples in which quantum annealers exhibit clear superiority over their classical counterparts. This project supports new approaches to development and testing of the inner workings of quantum annealers that would in turn help understand how to optimally utilize the potential of quantum annealers. Positive outcomes of this research would constitute scientific and computational breakthroughs with far reaching practical applications for the field of computation as a whole and should also have immediate applications in numerous key fields of practical interest.

Title: Validation Simulations of Macroscopic Burning-plasma Dynamics

Principal Investigator: Jacob King, *Tech-X Corporation*

Co-Investigators: Andrea M. Garofalo (*General Atomics*), Eric D. Held (*Utah State U.*), Thomas G. Jenkins (*Tech-X Corporation*),Carl R. Sovinec (*U. Wisconsin-Madison*), Alan D. Turnbull (*General Atomics*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 40,000,000 processor hours

Research Summary
ITER, a large fusion experiment under construction in France in which the U.S. is a partner, will enable significant progress in demonstrating the feasibility of commercial fusion power generation as a means of meeting long-term world energy needs. The complexity and large investment of ITER research initiatives must be supported by complementary development of advanced, predictive computational models for fusion experiments, especially to study physical phenomena that might result in damage to the device.

This allocation supports research into understanding and avoiding off-normal events in ITER experiments that could damage the device. Validating computational models using current experiments (where it is much safer to explore the physics of off-normal events) allows subsequent extrapolation of the model to ITER parameters, enabling detailed predictions of its expected behavior and increasing its chances for success. Outcomes of this project will include greater insight into the underlying physics both of steady-state operational regimes for ITER-relevant magnetically confined plasmas, and of various nonlinear instabilities which may impede such steady-state operation.

Title: Validation of RAP/HRRR for the Wind Forecast Improvement Project II

Principal Investigator: Joe Olson, *NOAA- National Oceanic and Atmospheric Administration*

Co-Investigators: V. Rao Kotamarthi, *Argonne National Laboratory*

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 15,000,000 processor hours

Research Summary

The total wind energy capacity in the United States is now more than 5% of the total installed power production capacity, giving the US the largest installed wind energy capacity in the world. The DOE's goal is for wind energy to meet 20% of the country's total energy needs by 2020, which will require both a significant increase in total capacity, and optimizing the energy production from existing wind farms. A large portion of the available wind resources are in complex terrain in the western US. Using these resources effectively requires the ability to forecast wind in the 15 minute to several hour range, allowing optimization of wind farm operation and smooth integration into the electrical grid. Existing models, which have been highly effective over the smoother terrain of the central US, have not performed effectively in this complex terrain. The DOE EERE Wind Energy program, in collaboration with NOAA and DOE laboratories, has initiated the Wind Forecast Improvement Program (WFIP2). The goal of this program is to develop numerical weather prediction models to improve wind forecasts in regions of complex terrain. This involves improving the physical parameterizations used in two NOAA operational weather forecast models, the 13-km resolution Rapid Refresh (RAP) and 3-km High-Resolution Rapid Refresh (HRRR). These models are often used by electrical grid operators to forecast wind energy production from wind farms and integrate wind energy into the electrical grid. The ALCC allocation will be used to conduct the numerical experiments that lead to improved parameterization of the atmospheric boundary layer in the models and hence better forecasting capabilities in complex domain. These simulations will be validated through an 18-month data collection and model validation effort in collaboration with an industrial partner. These validated models will provide a valuable tool for planning and operating future wind energy projects in complex terrain such as mountains, forests, and coastlines.

Title: Delivering Advanced Modeling & Simulation for Nuclear Energy Applications

Principal Investigator: John Turner, *Oak Ridge National Laboratory*

Co-Investigators: Kevin Clarno (*ORNL*), Ben Collins (*ORNL*), Thomas E. Evans (*ORNL*), Stuart Slattery (*ORNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 75,000,000 processor hours

Research Summary

Important challenges for the performance of nuclear reactors include safety, capital costs, and nuclear waste reduction. Due to the enormous parameter space and high costs of experiments, modeling and simulation (M&S) is critical for addressing these challenges. The Consortium for Advanced Simulation of Light Water Reactors (CASL) is a U.S. Department of Energy (DOE) Energy Innovation Hub established for M&S of nuclear reactors. CASL applies existing M&S capabilities and develops advanced capabilities to create a new software environment for predictive simulation of light-water reactors (LWRs). This environment, the Virtual Environment for Reactor Applications (VERA), incorporates science-based models, advanced numerical methods, modern computational science and engineering practices, and uncertainty quantification (UQ). Data from operating pressurized water reactors (PWRs), single-effect experiments, and integral tests are used to validate VERA models and methods.

Building on the success of CASL since conception in 2010, this allocation supports an extension and expansion of VERA capabilities to a broader set of reactor types. The outcome will support three areas of nuclear power plant (NPP) performance: (1) reducing capital and operating costs by enabling power upgrades and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new NPPs, (2) reducing nuclear waste volume generated by enabling higher fuel burnup, and (3) enhancing safety by enabling high-fidelity predictive capability for component performance through the onset of failure. In addition, VERA is being deployed via Industry Test Stands with supporting documentation and tutorials so the broader nuclear reactor industry can benefit from CASL developments.

The outcome of this project will be increased predictive capabilities for the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics**.**

Title: Large Scale Ab-initio Simulation of Crystalline Defects in Mg-alloys

Principal Investigator: Kaushik Bhattacharya, *California Institute of Technology*

Co-Investigators: Michael Ortiz (*Caltech*), Mauricio Ponga (*Caltech*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 20,000,000 processor hours

Research Summary

A predictive understanding of materials properties would empower science and engineering in most every sector and is a primary goal of materials science research. One large and important category of materials are crystalline solids. Common examples include metals such as magnesium alloys, insulators, ice, and certain rocks. Important properties of crystalline solids are mediated through defects in the crystal structure. These defects can have large impacts even when the defect occurs very rarely (the defect is in dilute concentrations). Thus, a predictive understanding of material properties of crystalline solids requires an understanding of the defects. Unfortunately this is challenging, as defects intimately couple the small (sub-atom sized) and large scales: the complex chemistry of the broken bonds in the core, the discrete atomistic nature of the annular region, and the long-range slow decay of continuum elastic fields. Density functional theory (DFT) is a simulation method that models materials at the very small atomistic/electronic structure. DFT is necessary to study the small atom sized impacts of defects, but it is a great challenge to extend DFT to larger scales. Yet, to capture the full range of defect impacts on crystalline materials, this challenge must be overcome.

A number of multiscale approaches have been proposed to address this challenge, but these approached require asymptotic assumptions or ad hoc patches that require case specific expertise in their implementation. These are not only counter to the *ab initio* philosophy, but also restrict their transferability and their predictive ability.

This ASCR Leadership Computing Challenge project supports the peta-scale computation of materials properties from density functional theory. In contrast to previous methods, DFT is the sole input and controlled numerical approximations enable the study of detects at realistic concentrations. The project supports continued development of *MacroDFT*, the team's sub-linear scaling computational platform for applying density functional theory to crystalline solids with defects. The project will use MacroDFT to perform a systematic study of defects in Magnesium and its alloys. Mg-alloys have some of the highest strength-to-weight ratios amongst metals. Outcomes of this project can have a huge impact in new lightweight engineering applications and demonstrate a method for predicting materials properties in crystalline materials.

Title: Prediction of Morphology and Charge-transfer Properties in Bulk Material and at Donor/Acceptor Interfaces of Thin-film Organic Photovoltaic Cells

Principal Investigator: Kendall Houk, *University of California Los Angeles*

Co-Investigators: Neil K. Garg (*UCLA*), Yang Yang (*UCLA*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 40,000,000 processor hours

Research Summary

In order to accelerate independence from damaging and finite fossil fuels, it is necessary to develop clean and renewable energy sources that can support increasing worldwide demands. Solar cells convert sunlight into electricity and present an excellent alternative due to the abundance of energy in solar energy that strikes the earth – over 9000 times greater than the current energy needs of our planet. However, current mainstream technology for solar cells uses inorganic materials that are expensive and toxic. In comparison, solution-processable oligomeric organic photovoltaic (OPV) cells are inexpensive, tunable, and flexible. The drawbacks of OPVs are low power conversion efficiency (PCE) and low long-term durability. Further, the development of devices is largely performed by intuitive and empirical approaches.

This project supports computational simulations to increase theoretical understanding of oligomeric OPV device performance. Specifically, this project develops massive computational models with atomic-level precision to predict how molecular structure influences the packing of many electron-donor molecules with each other, and with electron-acceptor molecules at 'bulk heterojunction' interfaces. The improved theoretical understanding will enable prediction of OPV performance from molecular structure. Simulations can then be used to predict new and promising high-performance OPV devices. In collaboration with expert synthetic, fabrication, and characterization research groups, devices identified through theoretical simulation will be fabricated and experimentally tested. The outcome of this project will move us closer to commercial organic solar cells and advance renewable energy technology.

Title: Molecular Dynamics Studies of Biomass Degradation in Biofuel Production

Principal Investigator: Klaus Schulten, *University of Illinois Urbana-Champaign*

Co-Investigators: Rafael C. Bernardi, *Beckman Institute, Energy Biosciences Institute*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 20,000,000 processor hours

Research Summary
Biofuels are a well-known alternative to fossil fuels. First-generation biofuels, such as corn ethanol, derive their energy from the chemical bonds in plants that are easy to break down into new energy forms. However first generation biofuels have important limitations, such as competition with food production, high fertilization needs, and low energy yields per hectare of land. Scientists overcome these limitations by exploring new sources of biofuel, such as switchgrass, which is cheap, easy to grow, and does not compete with food-stock. However the production of second-generation biofuels is not yet cost-competitive. One primary reason for the market delay in adopting second-generation biofuels is the challenge of harvesting energy from cellulose. Cellulose is a type of plant matter and is a characteristic content of second-generation biofuels. The bonds in cellulose are particularly challenging to break (thus cellulose is not a source of calories for humans). However, many animals, such as termites and cows, are capable of breaking the bonds in cellulose and extracting energy. Inside the gut of these animals are special bacteria that can break apart cellulose using enzyme complexes called cellulosomes. If industry can successfully capitalize on the chemical processes of cellulosomes to break down cellulose for energy production, second generation biofuels could become market competitive.

This project supports molecular dynamics tools to investigate the cellulosomes at the molecular level. The project will address key problems of the biofuel industry, namely end product inhibition of glycoside hydrolases, glycosylation effect on enzymatic activity and the usage of synthetic polymers in cellulose fiber pretreatment. The outcome of this project will advance understanding of methods for breaking cellulose bonds and advance renewable energy goals of creating cost-effective renewable and clean energy.

Title: First Principles Large Scale Simulations of Interfaces for Energy Conversion and Storage

Principal Investigator: Marco Govoni, *University of Chicago and Argonne National Laboratory*

Co-Investigators: Christopher Knight, (*ANL*), Giulia Galli (*U. Chicago*), Francois Gygi (*UC Davis*), Jonathan Skone (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 75,000,000 processor hours

Research Summary
The search for new materials that can extract, convert and store energy with greater efficiency represents a grand challenge of basic energy sciences. Whether the aim is finding efficient light absorbers for fuel production from water or high energy density rechargeable batteries, the solid/liquid interface plays a decisive role in modulating the photo-electro-chemical reactions responsible for the device operation.

This project supports application of large-scale quantum simulation methods to the solid/liquid interfacial region pertaining to renewable energy applications, including solar powered fuel production, and electrical energy storage. The study will employ *ab initio* molecular dynamics simulations to obtain atomic trajectories and compute ensemble averages and thermodynamic properties, and Many Body Perturbation Theory to compute accurate band edges and spectroscopy signatures of solid/liquid interfaces. Our highly scalable codes are capable of tackling systems of unprecedented size (several thousands of electrons).

The specific aims of the project are: (i) to provide knowledge and computational tools to interpret the large body of current experiments on fuel production from water and high density electrical energy storage; and (ii) to establish design rules for predicting Earth abundant, non-toxic, photo-electrodes with interfacial properties optimally suited to either extract, convert or store energy.

The high-performance modeling of the photo-electro-chemical processes that govern the efficiency of energy conversion and storage device operations will advance functional materials optimization and renewable energy technologies.

Title: Large Eddy Simulation and Direct Numerical Simulation of Fluid Induced Loads on Reactor Vessel Internals

Principal Investigator: Milorad Dzodzo, *Westinghouse*

Co-Investigators: Gregory Meyer (*Westinghouse Electric*), Yiban Xu (*Westinghouse Electric*), Emre Tatli (*Westinghouse Electric*), Teresa Bissett (*Westinghouse Electric*), Elia Merzari (*ANL*), Aleksandr Obabko (*ANL*), Oana Marin (*ANL*), Paul Fischer (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 40,000,000 processor hours

Research Summary
Understanding the loads on components within the nuclear reactor vessel, also known as Reactor Vessel Internals (RVI's), is crucial to proper structural design of these components. Predicting the loads created by the turbulent flow of coolant over individual reactor components is a particularly challenging problem. Currently, these loads are estimated extremely conservatively to ensure structural robustness, and used to calculate forcing functions that are then used to design components. Increasing the accuracy of these calculations will improve the best estimate calculations related to uncertainty management for safety margin quantification and associated structural margin recapture evaluations. This information is needed for aging management, life extension and reactor safety evaluations. To obtain the increased accuracy required, simulations of the fluid flow over a circular cylinder will be performed using two advanced Computational Fluid Dynamics (CFD) models for turbulence simulation: Large Eddy Simulation (LES) and the more computionally intensive Direct Numerical Simulation (DNS). The results will be compared with existing experimental results for unsteady lift and drag over a cylinder. These are the conditions typically used for RVI cross-flow calculations for multiple geometries and components, including safety related core support structures. If successful, the developed and validated tool set would allow the follow on work and comparison with other data sets relevant for RVI's, and more accurate prediction of the loads on these structures.

Title: Computational Design of Interfaces for Photovoltaics

Principal Investigator: Noa Marom, *Tulane University*

Co-Investigators: Volker Blum (*Duke University*), Oliver T. Hofmann (TU *Graz ,Austria*), Hong Li (*Georgia Tech*), Thomas Körzdörfer (*U. Potsdam, Germany*), Christian Ratsch (*UCLA*), Patrick Rinke (*Aalto Unviersit, Finland*), Chad Risko (*U. Kentucky*), Alvaro Vazquez-Mayagoitia (*ANL*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	100,000,000 processor hours
Site:	Lawrence Berkeley National Laboratory
Allocation:	20,000,000 processor hours

Research Summary

The functionality and efficiency of electronic devices, such as solar cells, are often determined by interactions at the interface between two materials. Here, novel computational algorithms will be developed and implemented to conduct large-scale, massively parallel quantum mechanical (first principles) and molecular-dynamics simulations to probe the physical attributes of critical interfaces in promising solar cell technologies, with particular focus on applications where the active layer is composed of either organic, hybrid organic-inorganic, or layered inorganic materials. These algorithms and simulation protocols will advance the current state-of-the-art in first-principles and multiscale simulations, and allow us to reveal essential details of these interfaces that are difficult to resolve experimentally. The theoretical understanding developed in this project will allow for new design paradigms to emerge for next-generation solar cell technologies.

Title: Delivering the Department of Energy's Next-generation High Resolution Earth System Model

Principal Investigator: Peter Thornton, *Oak Ridge National Laboratory*

Co-Investigators: David Bader (*LLNL*), William Collins (*LBNL*), Robert Jacob (*ANL*), Mark Taylor (*SNL*), Philip Jones (*LANL*), Philip Rasch (*PNNL*), Dean Williams (*LLNL*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	110,000,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	55,000,000 processor hours

Research Summary

Earth's climate is dependent on many complex sub-systems including clouds, aerosols, sea-ice, land-ice, ocean, land hydrology, land/ocean biogeochemistry and human activity. The goal of the Accelerated Climate Model for Energy (ACME) is to improve the current models for each sub-system and connect them into a full model for Earth's climate. The ACME goal requires multidisciplinary expertise and a large effort to bring into a single framework Earth's multi-scale multi-physics systems.

This project supports a large and multi-disciplinary team of Earth systems scientists, computational scientists, and software engineers in the development of a next-generation Earth system model. These scientists are improving the ACME model by including fundamental scientific advances in all of its component models. Science advances include the introduction of sub-grid representation for temperature and precipitation, high-resolution atmosphere with advanced cloud and aerosol parameterizations, and coupled thermal-hydrology-biogeochemistry in the land subsurface. The project also leverages large experimental and observational investments being made in DOE's Office of Science, Biological and Environmental Research Division to understand land ecosystems and improve their representation in high resolution Earth system models. The new model is designed to answer several pressing climate prediction science questions, and the current proposal provides the second year of compute resources needed to carry out the high-risk, high-payoff development.

Title: Developing Hyper-catalytic Enzymes for Renewable Energy

Principal Investigator: Pratul Agarwal, *Oak Ridge National Laboratory*

Co-Investigators: Chakra Chennubhotla (*University of Pittsburgh*), Nicolas Doucet (*INRS/University of Quebec*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 25,000,000 processor hours

Research Summary

Biofuels are a renewable energy source that can power gas and diesel engines from the energy stored in the chemical bonds of plant matter. One type of plant matter is 'cellulose' which forms the structural component of plants. The chemical bonds within cellulose hold a large amount of energy and cellulose is not a calorie source (to humans), making it an ideal source for biofuels. Yet large scale industrial production of biofuels from cellulose is not currently economical. One of the main reasons industry cannot mass-produce biofuel from cellulose is a lack of good catalysts. Catalysts are responsible for speeding up chemical reactions. Without catalysts, the chemical reactions needed to turn cellulose into biofuel are too slow for cost effective industrial production of biofuels. Engineering good catalysts for biofuel production from plant cellulose would enable industrial production of biofuel from cellulose and mark a significant step forward in renewable energy technology.

Enzymes are naturally occuring biological catalysts and are promising targets to engineer high efficient catalysts for cellulose based biofuel production. Computational simulations driven enzyme optimization techniques have shown great promise for developing highly efficient enzymes. This project supports a computational-experimental team developing high-quality predictive models of enzyme catalysis. Computational simulations coupled with experiments will yield fundamental insights into how enzymes work, with emphasis on identifying factors that can be used as enzyme engineering parameters. The development of these models has important implications, as it allows development of highly efficient enzymes that can be used at industrial scale at significantly reduced costs. For example, the team's ongoing work has already demonstrated the development of a hyper-catalytic prototypical enzyme showing 3000% improvement. This project supports simulations to enable a low-cost approach to developing highly efficient enzymes that can be used for industrial level production of cellulosic ethanol.

Title: Probing Novel Physics using Nucleon Matrix Elements

Principal Investigator: Rajan Gupta, *Los Alamos National Laboratory*

Co-Investigators: Tanmoy Bhattacharya (*LANL*), Vincenzo Cirigliano (*LANL*), Balint Joo (*Jefferson Lab*), Huey-Wen Lin (*U.C. Berkeley*), Kostas Orginos (*College of William and Mary*), David Richards (*Jefferson Lab*), Andre Walker-Loud (*College of William and Mary*), Frank Winter (*Jefferson Lab*), Boram Yoon (*LANL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 150,000,000 processor hours

Research Summary
Understanding the properties of fundamental particles that determine all behavior in the universe is a primary goal of physics. Protons and neutrons are composite particles (composed of quarks and gluons) that are the building blocks of all elements of the periodic table and are key-actors in the nuclear and chemical reactions that occur throughout the universe. Because of the importance of protons and neutrons, mapping the connection between quarks and gluons to the resulting properties of protons and neutrons represents a large piece of the ultimate goal of understanding the universe in terms of fundamental particles. This project supports investigation into the predicted properties of protons and neutrons from the theory that describes quarks and gluons (Quantum Chromodynamics). The high-precision calculations will enable theoretical interpretation of several experiments in nuclear and high energy physics that are being carried out in the US and at research centers all over the world. Specifically, this work will (i) explore new sources of the violation of an almost exact symmetry of nature called charge-parity (CP), (ii) extend the physics reach of measurements of the electric dipole moment of the neutron and put constraints on theories beyond the standard model being explored in the LHC at CERN, (iii) interpret high precision measurements probing tiny asymmetries in the decay of a neutron and (iv) provide calculations needed to improve estimates of how neutrinos interact with matter in experiments at Fermilab and other centers exploring neutrino oscillations. The outcome of this work will increase our understanding of protons and neutrons, improve the scientific precision and interpretation of experiments world-wide, and advance the exploration of new physics.

Title: Multi-Scale Modeling of Rotating Stall & Geometric Optimization

Principal Investigator: Ravi Srinivasan, *Dresser-Rand*

Co-Investigators: Logan Sailer (*Dresser-Rand*), Alain Demeulenaere (*Numeca*), David Gutzwiller (*Numeca*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 47,000,000 processor hours

Research Summary

Reducing greenhouse gas emissions from electrical power generation is one of the greatest engineering challenges for the 21st century. Because fossil fuels are expected to continue to play a large role in electrical production until at least 2050, methods for capturing and storing carbon dioxide in cost-effective manner are urgently needed. The Department of Energy currently sponsors large- scale demonstration projects to prove the viability of carbon capture and sequestration (CCS). A major technical challenge in CCS is compressing the carbon dioxide after it is captured. Dresser-Rand (D-R) is developing advanced high-pressure ratio single stage compression technology to reduce the cost of carbon dioxide compression.

Dresser-Rand has previously used Titan to simulate carbon dioxide compression technology, and will test first-generation compression technology based on these results in 2015. The current work focuses on the multi-scale modeling of rotating stall in a centrifugal compressor and the advancement of the next generation of CCS compression technology by generating optimized designs of the existing compressor geometry. D-R has demonstrated effective leadership-scale computing on the Titan system through intelligently driven optimizations. The rapid development of new compressor designs is a salient example of the exceptional capabilities provided through the ALCC project, and the incredible scientific and industrial opportunities enabled by the conjunction of high-performance computing and large scale optimization methods.

Title: Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral *Ab Initio* Study

Principal Investigator: Robert A. DiStasio, *Princeton University*

Co-Investigators: Biswajit Santra (*Princeton U.*), Fausto Martelli (*Princeton U.*), Hsin-Yu Ko (*Princeton U.*), Xifan Wu (*Temple U.*), Michele Ceriotti (*EPFL (Switzerland)*), Annabella Selloni (*Princeton U.*), Roberto Car (*Princeton U.*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 175,000,000 processor hours

Research Summary
A highly accurate and detailed understanding of the microscopic structure of liquid water is of great importance to a number of fields, ranging from biology/biochemistry to energy storage and electrochemistry. Several key properties of water, are crucial for understanding and predicting its role on Earth and in living systems. For instance, the density of water in the liquid, gas, and solid states is not what would be typically predicted. While most substances become less dense with rising temperatures, frozen water (ice) floats in warmer water. As such, a fundamental understanding of the anomalous density properties of water are critical to elucidating the role played by water in Earth ecosystems.

Another key property of water is the ability of a given water molecule (H2O) to transfer protons (a hydrogen atom with no electron, H+). Hydrogen atoms (H+) can be exchanged among H2O molecules forming the OH- and H3O+ ions. The ability of water to transfer protons is critical not only to the physical properties of water systems (e.g., oceans and rivers) but also to how biomolecules, including DNA and proteins, behave and work inside cells.

This project supports accurate theoretical determinations of the microscopic structure and properties of liquid water. This work will utilize highly accurate state-of-the-art ab initio molecular dynamics (AIMD) simulations in conjunction with large-scale massively parallel computer architectures to investigate the aforementioned properties of liquid water including its anomalous density properties and the proton transfer mechanisms in the formation of the hydronium (H30+) and hydroxide (OH-) ions. The outcome of this project will be an improved physical understanding of water, aiding advancements across a broad range of scientific and technological research frontiers.

Title: In Search of the Elusive Glue of Quantum Chromodynamics

Principal Investigator: Robert Edwards, *Jefferson Laboratory*

Co-Investigators: Jozef Dudek (*Old Dominion University and Jefferson Lab*), Balint Joo (*Jefferson Laboratory*), David Richards (*Jefferson Laboratory*), Frank Winter (*Jefferson Laboratory*), David Wilson (*Old Dominion University and Jefferson Lab*), Nilmani Mathur (*Tata Institute, Mumbai, India*), Mike Peardon (*Trinity College, Dublin, Ireland*), Sinead Ryan (*Trinity College, Dublin, Ireland*), Sinead Ryan (*Trinity College, Dublin, Ireland*), Christopher Thomas (*DAMTP, Cambridge University, Cambridge, UK*), Graham Moir (*University of Wuppertal, Germany*), Steve Wallace (*University of Maryland*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 50,000,000 processor hours

Research Summary

What particles can the universe create? Predicting theoretically and detecting experimentally all such particles is a fundamental goal of particle physics. The Standard Model (SM) predicts and explains the origin of many fundamental particles and their ability to become building blocks for larger forms of matter. Quarks are one group of fundamental particles found in the SM. The SM describes and predicts quark behavior using a theory called 'Quantum Chromodynamics' (QCD). QCD accurately predicts the three quark system of the more well-known proton and neutron (found in the nuclei of atoms) as well as a two quark system called a meson. QCD, however also predicts new exotic two quark pairings called 'exotic mesons' that as of yet, have never been observed. Determining if QCD predictions are correct and if the universe can indeed create exotic mesons would be a great discovery for science.

Thomas Jefferson National Accelerator Facility is undergoing an exciting upgrade that will enable the experimental facility to seek out new exotic meson states. A large challenge in the experimental search is that the exotic mesons would not be detected directly. Exotic mesons would rapidly decay and the pattern of the detected decay products is what marks their presence. To interpret decay-product detection, QCD theory of exotic mesons must be used to simulate and predict exotic meson behavior and decay. This project supports the computational implementation of QCD theory to determine the excited meson state and predict the preferred decay products of these excited states. The results will increase understanding of the predictions of QCD, improve utilization of the Jefferson facility, and further enable detection of new particles that may exist (albeit briefly) in our universe.

Title: Demonstration of the Scalability of Programming Environments By Simulating Multi-Scale Applications

Principal Investigator: Robert Voigt, *Leidos Inc.*

Co-Investigators: S. Balachandar (*U. Florida*), Jonathan Freund (*U. Illimois Urbana Champaign*), Karel Matous (*U. Notre Dame*), Gianluca Iaccarino (*Stanford University*), Lawrence Rauchwerger (*Texam A&M*), Martin Berzins (*U. Utah*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	127,000,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	40,000,000 processor hours

Research Summary

Effective use of high performance computing is an essential component of the US economy and national defense. Future computing systems leading to exascale will pose new challenges if they are to be used effectively to simulate complex applications that support the national interest. These systems introduce complexity to processor and system design not previously encountered. This effort brings together six leading universities conducting research leading to software that will support a spectrum of multiscale applications. A key component of the effort is to demonstrate the infrastructure required by these emerging architectures on these applications that include:

- **University of Florida:** Compressible multiphase turbulence resulting from explosions such as a volcanic eruption.
- **Univesity of Illinois:** Plasma coupled combustion in ignition of fuel in, for example, automobile engines.
- **Uniersity of Notre Dame:** The impact of shocks on heterogeneous materials.
- **Stanford University:** The effect of radiation on particle motion in a turbulent airflow in solar thermal receivers with applications in energy production.
- **Texas A&M University:** Radiation transport in nuclear reactor design and astrophysics.
- **University of Utah**: The simulation of large clean-coal boilers leading to clean generation of electricity.

This allocation supports development of software tools in the stated areas. This multi-institutional research project will advance effective use of high performance computing for a broad base of important scientific and technological areas.

Title: Hobbes: Operating System and Runtime Research for Extreme Scale

Principal Investigator: Ron Brightwell, *Sandia National Laboratories*

Co-Investigators: Terry Jones (*ORNL*), Patrick Bridges (*University of New Mexico*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 30,000,000 processor hours

Research Summary
Four key challenges facing future large-scale computing systems are: (1) dramatically improve power efficiency; (2) improve resilience in the presence of increasing faults; (3) enable efficient data movement across deepening memory hierarchies and new storage technologies; (4) managing dramatically increased parallelism. To address these challenges, the operating system and runtime (OS/R) must take on more responsibility for managing more resources, like power and parallelism, and share more of the burden for insulating applications from the complexities of a system. Much of the focus of extreme-scale system software in the last decade has been on measuring and characterizing the impact the operating system can have on application scalability. The Hobbes project is a collaboration of four national laboratories and eight universities with the goal of providing a system software environment that comprehensively exploits two technologies deemed critical for future supercomputing: application composition and lightweight virtualization. Application composition enables applications to be coupled efficiently without such constraints as a single runtime system. Lightweight virtualization provides the appearance of desired computer resources without the need of the actual resource. Rather than providing a single unified OS/R that supports several parallel programming models, Hobbes is leveraging lightweight virtualization that provides the flexibility to construct and execute custom OS/R environments. Evaluating the scalability of OS/R interfaces and mechanisms at large scale is crucial to Hobbes research and development. This project supports large scale testing and evaluation of OS/R implementation techniques to improve OS/R for future high performance computing machines.

Title: XPRESS Program Environment Testing at Scale

Principal Investigator: Ron Brightwell, *Sandia National Laboratories*

Co-Investigators: Thomas Sterling (*Indiana University*), Andrew Lumsdaine (*Indiana University*), Alice Koniges (*LBNL*), Hartmut Kaiser (*Louisiana State U.*), Tom Evans, (*ORNL*), Barbara Chapman (*U. of Houston*), Allan Porterfield (*U. of North Carolina/RENCI*), Allen Malony (*U. Oregon*), Allen Malony (*U. Oregon*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 27,000,000 processor hours

Research Summary

The eXascale Programming Environment and System Software (XPRESS) Project is one of the major Department of Energy (DOE) initiatives for advancing towards exascale (one million trillion calculations per second) computing. Its goal is to explore a means of dramatically improving efficiency and scalability through a set of guiding and interrelated operational and structural principles that together comprise an advanced execution model. This execution model is based on a fully dynamic and adaptive paradigm to exploit the capabilities of future generation performance oriented runtime systems and hardware architecture enhancements. We are also developing an associated programming model that enables fine---grained constraint based parallelism, and supports run-time adaptive resource management. We are using these models for a series of DOE miniapps, benchmark codes and full applications. The applications span a wide variety of DOE areas and hold differing programming model challenges. Many of the applications already have traditional data communication implementations, e.g., MPI + OpenMP, and several have been tested on platforms with large numbers of GPUs (graphics processing units). This request for computer time will enable comparison of conventional models with our new lightweight threaded approach to parallel programming. Additional XPRESS-- related end---to---end development paths include tools for profiling and runtime adaptation, accuracy, energy measurement, and legacy code migration techniques for the full programming environment.

Title: ALCC: Cosmic Frontier Computational End-Station

Principal Investigator: Salman Habib, *Argonne National Laboratory*

Co-Investigators: Julian Borrill (*LBNL*), Karin Heitmann (*ANL*), Nick Gnedin (*FNAL*), Zarija Lukic (*LBNL*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	65,000,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	35,000,000 processor hours
Site:	Lawrence Berkeley National Laboratory
Allocation:	15,000,000 processor hours

Research Summary

The Cosmic Frontier effort within DOE HEP targets the physics of dark energy and dark matter, cosmological probes of neutrino physics, and the nature of primordial fluctuations – some of the most exciting problems in all of physical science. Powerful cosmological surveys are essential components of a major national and international research program in these areas. DOE-supported experiments include the Dark Energy Survey (DES) and the South Pole Telescope (SPT). Planned future surveys include the Dark Energy Spectroscopic Instrument (DESI), the Large Synoptic Survey Telescope (LSST), and SPT-3G. Simulations and data analyses play a central role in interpreting observations, and cross-correlation analyses across different types of measurements are necessary to develop new measurement methods and to control systematic errors. Motivated by these considerations, this allocation supports a computational end-station tasked with an initial set of simulation and analysis sub-projects. Because numerical simulations are essential for making theoretical predictions and analyzing observations, it is important to bring experts in their respective specializations under a single umbrella – the end-station – in order to establish a computational program that can properly address the diverse set of issues involved. Additionally, the observational community needs to be more directly involved in analyzing simulations, because simulations provide important routes – sometimes the only routes – to understanding and controlling many of the problems touched upon above.

Title: Enabling Next-Generation Light Source Data Analysis through Massive Parallelism

Principal Investigator: Xiaoye Sherry Li, *Lawrence Berkeley National Laboratory*

Co-Investigators: Abhinav Sarje, (*LBNL*), Alexander Hexemer, (*LBNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 10,000,000 processor hours

Research Summary

Thin films are a class of material characterized by nanometer to micrometer thickness and are key components to the design and fabrication of energy-relevant nanodevices, such as photovoltaics, energy storage systems, batteries, fuel, and carbon capture and sequestration devices. Understanding the detailed morphology of thin-film surfaces is of high value to an array of energy technologies. Grazing Incidence Small Angle X-ray Scattering (GISAXS), is one important experimental method that allows scientists to understand thin-film surfaces at nanoscopic levels of detail. However, at present, there is no robust software to deduce the precise shapes and geometric features of the nanoparticles ensemble from the GISAXS output data. One of the large challenges in this process is the "parameter fitting" required for the sample. In probing complex structures, a model definition can grow as large as a 3D grid with billions of cells – a very computationally intensive challenge that existing single-node analysis tools cannot handle.

Our recent developments have resulted in a high-performance software, HipGISAXS, with basic simulation capabilities able to utilize massively parallel systems with several hundreds of thousand cores. This project supports enhancements of HipGISAXS to include inverse modeling capabilities, development of a robust and efficient framework for parameter fitting, including randomized nonlinear least squares methods, surrogate model methods, particle swarm methods, and reverse Monte Carlo methods. The outcome of the project will enable insights and discoveries in into important energy material structures at the level of nanoscale.

Title: Advancing Internal Combustion Engine Simulations Using Sensitivity Analysis

Principal Investigator: Sibendu Som, *Argonne National Laboratory*

Co-Investigators: Peter Kelly Senecal (*Convergent Science Inc.*), Marta Garcia Martinez (*ANL*), Albert Wagner (*ANL*), Janardhan Kodavasal (*ANL*), Yuanjiang Pei (*ANL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory

Allocation: 60,000,000 processor hours

Research Summary

The overwhelming majority of cars, buses, and trucks on the road today are powered by Internal Combustion (IC) engines, using a mixture of fossil fuels and biofuels. Because these vehicles are expected to remain as the primary mode of transportation worldwide for the foreseeable future, optimizing their design will have a large impact on reducing pollution. Traditionally, IC engines are designed based on expensive and time-consuming experimental testing. Simulation using High Performance Computing (HPC) offers the opportunity to both reduce testing, and to obtain new physical insights into IC engine operation. HPC simulations of IC engines are challenging: multiple processes, including chemistry, spray dynamics, turbulent fluid mechanics, and heat transfer must all be simulated accurately to determine the performance and emissions characteristics of an engine. These processes must be simulated across multiple length and time scales. Current simulations are performed on small clusters, and the results are extremely sensitive to the grid used in the calculation.

The current work will use the supercomputer Mira to perform high-fidelity simulations that incorporate uncertainty analysis for input parameters such as physical, boundary conditions, model, and chemical kinetics. Using powerful computational resources, IC engine simulations can achieve grid convergence, thus reducing significant uncertainty in the calculations. Furthermore, Global Sensitivity Analysis (GSA) will be performed on the data obtained from thousands of simulations for a variety of input parameter uncertainties as identified above. GSA will help identify critical model, chemical kinetic, and boundary condition uncertainties for simulations, and in turn provide unique insights into IC engine simulation and operation.

Title: Fluctuations of Conserved Charges in High Temperature QCD

Principal Investigator: Swagato Mukherjee, *Brookhaven National Laboratory*

Co-Investigators: F. Karsch (*BNL*), E. Laermann (*Bielefeld University, Germany)*, P. Petreczky (*BNL*), C. Schmidt (*Bielefeld University, Germany)*, S. Sharma (*BNL*), M. Wagner (*Indiana University*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 167,000,000 processor hours

Research Summary

Solids, liquids, and gasses are three examples of "phases" of matter. The phase of a substance, such as liquid water vs water ice, is determined by variables such as the temperature and pressure. A diagram of a substance's phase versus temperature and pressure (for example) is known as a phase diagram. Phase diagrams can show a surprisingly rich set of phases; ordinary H_2O, for example, is believed to support at least 15 different phases of ice, characterized by different internal arrangements of the H_2O molecules. Knowing the phase diagram is a crucial step towards understanding the properties of a material, and is often useful in developing real-world applications.

The more exotic "nuclear matter" in atomic nuclei is also described by a phase diagram. Nuclei are made of strongly interacting protons and neutrons, which are themselves composed of quarks, bound together by gluons. Just as ice melts into water when sufficient energy is added to raise the temperature to the melting point, so the protons and neutrons in nuclei can "melt" into a remarkable phase of matter with liberated quarks and gluons, the "quark gluon plasma" (QGP), when energy is added through high velocity collisions of nuclei. Establishing the boundary between atomic nuclei and the QGP in the nuclear matter phase diagram is a central goal of the heavy-ion research programs at major experimental facilities such as the Relativistic Heavy Ion Collider (RHIC) at BNL and ALICE at CERN.

As the theory that describes quarks and gluons, Quantum Chromodynamics (QCD), is precisely known mathematically and can be studied on supercomputers, one might hope to predict the phase diagram of QCD directly. This can already be done for gluons alone, but determining the phase diagram of the real-world mixture of quarks and gluons requires new computational techniques. This ALCC project supports the investigation of a promising method for predicting the QCD phase diagram in the presence of both quarks and gluons. A special goal of this research is to attempt to find the conjectured "critical point" in the QCD phase diagram, the end point of the line along which nuclei and the QGP phase coexist . The results of this project are expected to help in the interpretation of experimental observations at RHIC, and to contribute to our understanding of the physics of quarks and gluons more generally.

Title: Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions

Principal Investigator: Thomas Blum, *University of Connecticut*

Co-Investigators: Norman Christ (*Columbia U.*), Masashi Hayakawa (*Nagoya U. (Japan)*), Tomomi Ishikawa (*RBRC/BNL*), Taku Izubuchi (*BNL*), Luchang Jin (*Columbia U.*), Christoph Lehner (*BNL*), Norikazu Yamada (*KEK (Japan)*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 175,000,000 processor hours

Research Summary

There are four fundamental forces, or interactions, in Nature: the familiar gravity and electricity and magnetism, and the less familiar weak and strong forces. These forces (excluding gravity), along with all of the known fundamental particles, form the Standard Model (SM) of particle physics, our most basic theory. The SM is one of the greatest achievements of Science, yet physicists know it is incomplete. This has led to a worldwide challenge, the search for new physics, or extensions of the SM.

The magnetic moment of the muon, which acts like a tiny compass needle, is a sensitive probe of the SM and its possible extensions, which may include undiscovered particles, or even new forces. Physicists have measured, to incredible precision (0.54 ppm), how the muon wiggles, due to its moment, when placed in a magnetic field. Theorists have calculated what the moment should be, to even better precision, but the two don't quite agree.

To tell whether there must be new physics, or not, a new experiment will be done soon at Fermilab (and hopefully at J-PARC in Japan). But for the new comparison to be successful, the theory must improve too. The biggest uncertainty comes from the hadronic contributions, arising from the strong force, also known as quantum chromodynamics (QCD). To solve QCD with the required precision takes enormous compute resources. The aim of this project is to calculate the so-called hadronic light-by-light scattering contribution, using a numerical framework called Lattice QCD to solve the underlying quantum field theory.

Title: Modeling RF-induced Sheath Effects and Parasitic Losses In Magnetic Fusion Experiments

Principal Investigator: Thomas G. Jenkins, *Tech-X Corporation*

Co-Investigators: David N. Smithe (*Tech-X Corporation*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 48,000,000 processor hours

Research Summary

Fusion technology holds promise as a nearly limitless supply of renewable energy that can meet the world's energy demand. International collaborative efforts to this end are presently focused on the multibillion-dollar ITER device, which uses magnetic fields to confine the superheated, ionized gas (plasma) needed for the fusion reaction. Highly challenging scientific and engineering barriers must be overcome to control and harness fusion energy from magnetically confined plasmas. Energy production in magnetic fusion reactors is enabled by radiofrequency antennas, which heat confined plasma to the high temperatures needed for fusion reactions to occur. However, narrow "plasma sheaths" form very near the antenna and other material surfaces, and introduce a host of complex physics effects. Particles accelerated through the strong electromagnetic fields of the sheath collide with wall surfaces, and may release impurities that contaminate the fusion reaction. As well, under certain conditions a portion of the radiofrequency heating power may also be diverted to excite undesired waves near the plasma edge, giving rise to reduced reactor efficiencies since this power is effectively wasted.

This project supports computational investigation of the physics underlying inefficiencies that arise from plasma sheaths and undesired wave excitation in the plasma edge. Using recently developed approaches for the numerical modeling of sheath behavior and wave excitation, we will explore the physics underlying these effects by modeling antenna operation in realistic experimental scenarios. We will validate these physics simulations by comparing our results against experimental data from the Alcator C-Mod experiment, and will quantify the conditions under which the undesirable impurity production and wave excitation effects occur. The project will also investigate possible techniques to mitigate such impurity production and wave excitation in existing fusion experiments, and will explore the ramifications of the underlying physics effects and the developed mitigation techniques for future fusion experiments such as ITER.

Title: An End-Station for Intensity and Energy Frontier Experiments and Calculations

Principal Investigator: Thomas LeCompte, *Argonne National Laboratory*

Co-Investigators: Paolo Calafiura (*LBNL*), Craig Tull (*LBNL*), Brendan Casey (*Fermi NAL*), J. Taylor Childers (*ANL*), Stefan Hoeche (*SLAC*), Alexei Klimentov, Torre Wenaus (*BNL*), Thomas D. Uram, Venkat Vishwanath (*ANL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory
Allocation: 62,000,000 processor hours
Site: Lawrence Berkeley National Laboratory
Allocation: 16,000,000 processor hours

Research Summary

High Energy Physics studies the properties of matter, energy, space and time at the smallest possible distances. We do this by building particle detectors of great size and complexity – in some cases weighing thousands of tons and having millions of readouts. We then use these detectors by comparing computer simulations of what we would expect to see if different theories hold true with the actual data, and seeing which, if any, match. Progress can be made by improving either end of this comparison, and we propose here to improve the quality of the computer simulation. Using supercomputers, we can produce more simulated events, and simulation events of better accuracy or greater complexity than we could otherwise.

This project supports a team of experimental and theoretical physicists working together to answer fundamental questions for High Energy Physics. While much of the work is unique to each project, much of it is in common, and by working together we can accomplish more than we can by ourselves. Additionally, by working together, we have created an environment where other particle physicists can use these supercomputers more easily and quickly than they would on their own, to the benefit of everyone.

Title: Portable Application Development for Next Generation Supercomputer Architectures

Principal Investigator: Tjerk Straatsma, *Oak Ridge National Laboratory*

Co-Investigators: Katie Antypas (*NERSC-LBNL*), Timothy Williams (*Argonne*)

ALCC allocation: Processor Hours

Site:	Argonne National Laboratory
Allocation:	60,000,000 processor hours
Site:	Oak Ridge National Laboratory
Allocation:	60,000,000 processor hours
Site:	Lawrence Berkeley National Laboratory
Allocation:	40,000,000 processor hours

Research Summary

Supercomputers are powerful scientific and mathematical instruments capable of calculating quadrillions of operations in a single second. Science harnesses the compute speed of supercomputers to tackle some of science's biggest challenges including exploration of complex and important theories, simulation of otherwise impossible experiments on sub-atomic to cosmological scales, and rapid prototyping to speed time-to-solution for industrial technology. Although supercomputers can significantly advance science and technology, a great barrier to benefitting from supercomputers exists in the challenge of programming application software that is capable of using these massively parallel systems.

Three science driven DOE supercomputing facilities; Argonne Leadership Computing Facility (ALCF), National Energy Research Scientific Computing Center (NERSC) and the Oak Ridge Leadership Computing Center (OLCF), are supporting efforts to prepare scientists and engineers for the next-generation supercomputers that are planned for these centers through early application readiness programs that will prepare a range of application codes. The ALCF has the Early Science Program (ESP), NERSC the NERSC Exascale Science Application Program (NESAP), and the OLCF, the Center for Accelerated Application Readiness (CAAR) program.

This allocation supports these three facilities as they launch these application readiness programs addressing 40 key application codes. In order for the application readiness programs to be successful it is crucial that application developers have allocations not only at their sponsored supercomputing facility, but also at a facility with an alternate architecture so portability issues can be explored. This project will support the computational resources on the current systems to start this collaborative effort and help scientists and engineers leverage future HPC systems.

Title: Multi-Neutron Forces from QCD

Principal Investigator: William Detmold, *Massachusetts Institute of Technology*

Co-Investigators: Silas R. Beane (*U. Washington*), Kostas Orginos (*College of William and Mary, Jlab*), Martin Savage (*Institute for Nuclear Theory*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 52,000,000 processor hours

Research Summary

Isotopes are elements whose nucleus has the same number of protons but different numbers of neutrons. Although neutrons are uncharged, even a small change in neutron number can significantly alter the properties and behavior of a nucleus. For example, carbon-14 is radioactive while carbon-13, with one fewer neutron, is not. Understanding isotopic differences has led to huge scientific and technological advances such as carbon dating, nuclear energy, and medical imaging. To pursue greater understanding of isotopes and the physics of atomic nuclei, a new national user facility, the Facility for Rare Isotope Beams (FRIB), is under construction. FRIB will use high energy beams to create and study new isotopes that are not naturally found here on Earth. To understand and drive the experiments at FRIB, new and deeper theoretical understanding of, and predictions for, the behavior of nuclei must be developed.

This proposal supports calculations of properties of multi-neutron systems (e.g. systems with more than one neutron, either alone, or in combination with protons, such as in helium-6). To accurately capture the behavior and interactions of neutrons and protons, the calculations will work directly with quarks and gluons, the fundamental particles that combine to form neutrons. Quark and gluon dynamics are described using a theory called 'quantum chromodynamics (QCD)' and the results of these QCD calculations will be used to provide first principles constraints on the many-body forces between protons and nuetrons. These theoretical calculations will complement upcoming experimental measurements at FRIB, and will also have direct impact upon our understanding of neutron stars, one of the universe's natural high-energy experiments. The outcome of this project will be to refine our predictive capabilities in extreme astrophysical environments, optimize knowledge gained from FRIB, and enhance our understanding of multi-neutron forces.