**Title:** Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An Ab Initio Study of Liquid Water

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

**Co-Investigators:** David T. Limmer (*Princeton University*), Biswajit Santra (*Princeton University*), Fausto Martelli (*Princeton University*), Hsin-Yu Ko (*Princeton University*), Michele Ceriotti (*EPFL, Switzerland*), Annabella Selloni (*Princeton University*), Roberto Car (*Princeton University*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory

**Allocation:** 350,000,000 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. At present there is no experimental methodology available to directly obtain the real-space microscopic structure of liquid water. Computer-based simulations can provide this information in a relatively straightforward manner. However, the quality of computer-based predictions relies heavily upon the accuracy of the underlying potential used to describe the intra- and inter-molecular interactions present in liquid water. In this work, we seek to 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 structure of liquid water in three different and important aqueous environments: (1) dilute aqueous ionic solutions, (2) a catalytic metal-oxide interface, and (3) extreme aqueous environments. Each of these three environments represents drastically different underlying water structures. The outcome of this project will be an improved understanding of water which will aide advancements in a broad range of scientific and technological research frontiers.

**Title:** The Spectrum and Properties of Exotic Mesons in Quantum Chromodynamics

**Principal Investigator:** Robert Edwards, *Jefferson Laboratory*

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

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 250,000,000 processor hours

**Research Summary:**

Understanding mesons, a type of subatomic particle, is critical to advancing our knowledge of matter and fundamental physics. The determination of the meson spectrum is a world-wide effort and exploring the excited meson spectrum is a flagship project of the Thomas Jefferson National Accelerator Facility (Jefferson Lab) The excited meson spectrum is of particular interest because it may reveal important properties of “exotic” mesons. GlueX is a new experiment at Jefferson Lab built to discover and explore properties of exotic meson states. In this proposal, we will compute the excited-state meson spectrum of Quantum Chromodynamics (QCD), the theory of strong interactions (a fundamental force of nature). The goal of the computational research is to predict from theory and simulation the masses of possible exotic meson states in advance of the first experimental results from GlueX. These calculations will guide future experimental searches and advance our understanding of matter and fundamental physics.

**Title:** Applying Breakthroughs in Protein Structure Calculation to the Creation of Designer Enzymes

**Principal Investigator:** David Baker, *University of Washington*

**Co-Investigators:** Scott J. Miller (*Yale University*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory

**Allocation:** 200,000,000 processor hours

**Research Summary:**

Proteins are large molecules found in all living organisms that serve as the major functional units of all life. Proteins are made from a sequence of amino acid building blocks. Key to understanding proteins is to understand the relationship between the amino acid sequence, the three-dimensional folded structure, and the resulting protein function. The Baker laboratory has developed the Rosetta software suite for predicting protein structure given the amino acid sequence, and for designing amino acid sequences capable of folding into novel structures with desired functions. Of particular interest are enzymes, a type of protein responsible for catalyzing (aiding) chemical reactions. Enzymes serve as nature's bio-machinery and are responsible for invaluable functions such as converting food to energy, building cell walls, and repairing DNA. Recent advances in massively-parallel design algorithms have opened the door for the design of artificial enzymes capable of catalyzing chemical reactions that no natural enzyme can catalyze. Designer enzymes could have broad applicability in many DOE priority areas, such as sustainable domestic biofuel production, and could reduce energy consumption and improve energy efficiency by permitting industrial syntheses to occur at lower temperatures and with fewer unwanted byproducts. We propose to use a multi-state protein design strategy dependent on large scale parallel supercomputing hardware to create designer enzymes with a broad range of applications.

**Title:** Cosmic Frontier Computational End-Station

**Principal Investigator:** Salman Habib, *ANL*

**Co-Investigators:** Julian Borrill (*LBNL*), Nick Gnedin (*Fermilab*), Katrin Heitmann (*ANL*), Zarija Lukić (*LBNL*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 100,000,000 processor hours

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 76,000,000 processor hours

**Research Summary:**
The Cosmic Frontier effort within the Department of Energy Office of High Energy Physics targets the physics of dark energy and dark matter, cosmological probes of neutrino physics and the nature of primordial fluctuations - some of the most important questions in all of fundamental physical science. Cosmological surveys are essential components of a major national and international research program aimed at understanding these questions. Simulations and data analyses play a central role in interpreting observations, and cross-correlation analyses across different types of measurements are necessary to control systematic errors. Motivated by these considerations, this project will support a computational end-station tasked with an initial set of simulation and analysis sub-projects. Outcomes of this work will support interpretation of experimental data from cosmological surveys and further our understanding of fundamental physics.

**Title:** Validation Studies of Gyrokinetic Simulations to Understand the Coupling of Ion and Electron Scale Turbulence in Tokamak Plasmas

**Principal Investigator:** Christopher Holland, *University of California, San Diego*

**Co-Investigators:** N. T. Howard (*Oak Ridge Institute for Science and Education*), J. Candy (*General Atomics*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 90,000,000 processor hours

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 50,000,000 processor hours

**Research Summary:**
In order to realize the promise of nuclear fusion as an energy source, it is essential to develop predictive models of plasma dynamics that can accurately describe the performance of current experiments, and be confidently extrapolated to future devices. One of the essential processes such models must describe is the turbulent transport of plasma, which often determines the overall performance and fusion energy produced. Recent cutting-edge multiscale gyrokinetic simulations of plasma turbulence in a tokamak (the leading approach to magnetic confinement based fusion devices) have resolved previously observed discrepancies between the observed turbulence levels and those predicted by earlier simulations that included only a smaller range of spatial range of scales. This award will extend the direct multiscale simulation approach to a wider range of parameters and conditions. The results of these studies will significantly advance our understanding of plasma turbulence in tokamaks, and our ability to predict turbulent transport and confinement in future devices with greater accuracy and confidence.

**Title:** Delivering the Department of Energy's next-generation high-resolution Earth system model

**Principal Investigator:** Peter Thornton, *ORNL*

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

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 107,000,000 processor hours

**Site:** Oak Ridge National Laboratory
**Allocation:** 30,000,000 processor hours

**Research Summary:**
Predictive understanding of Earth's climate is of deep scientific interest and of great social relevance. A large multi-disciplinary team of Earth system science domain experts, computational scientists, and software engineers is tackling the development of a next-generation Earth system model with fundamental scientific advances in all of its component models. Science advances include the introduction of predictive human system components, high-resolution atmosphere with advanced cloud and aerosol parameterizations, coupled thermal-hydrology-biogeochemistry in the land subsurface and advanced disturbance dynamics for vegetation. The new model is designed to answer several pressing climate prediction science questions. This work supports the first year of compute resources needed to carry out the high-risk, high-payoff development, parameterization, and coupled system evaluation tasks required to move the project toward delivery of this new modeling system.

**Title:** Predictive Large-Eddy Simulation of Jet Fuel Atomization, High-Lift Airframes and Reacting Supersonic Turbulent Flows on Unstructured Grids

**Principal Investigator:** Parviz Moin, *Stanford University*

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

**Research Summary:**
Accurate predictive modeling is crucial in the design of energy-efficient and environmentally friendly engineering systems, including aircraft propulsion and land based power generation. High-fidelity, unstructured large-eddy simulation (LES) is emerging as an accurate yet cost-effective computational tool for prediction of several key aircraft components. Combining recent advances in LES modeling with our highly scalable, unstructured code CharLES, predictive LES of real aircraft geometries at flight Reynolds number is possible using today's leadership-class computers. Three high-risk, high-payoff simulations are examined that leverage the CharLES codebase to significantly advance the state-of-the-art in LES technology for (1) liquid jet atomization, (2) wall modeling and control of turbulent boundary layers, and (3) supersonic turbulent combustion flamelet modeling for hypersonic flight. This project aims to demonstrate that LES of complex geometries at flight Reynolds numbers is possible with today's large-scale computers, which is a crucial step towards extended use of LES in transportation and power industries.

**Title:** Interfaces in Organic and Hybrid Photovoltaics

**Principal Investigator:** Noa Marom, *Tulane University*

**Co-Investigators:** Volker Blum (*Duke University*), Jean-Luc Bredas (*Georgia Institute of Technology*), Jeff R. Hammond (*ALCF*), Thomas Korzdorfer (*University of Potsdam, Germany*), Patrick Rinke (*Fritz Haber Institute of the Max Planck Society, Germany*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 75,000,000 processor hours

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 30,000,000 processor hours

**Research Summary:**
Future technologies will require new paradigms in design, functionality, scalability and a reduction in power consumption to meet our global energy challenges and to reduce our environmental footprint. The quest for clean and sustainable energy sources has driven the development of solar cell technology. Organic photovoltaics (OPV) and dye-sensitized solar cells (DSCs) are particularly attractive for low cost, large area applications. In both types of solar cells, charge separation is achieved at an interface between two materials. This crucial step in the generation of the desired electrical current depends critically on the properties of the interface. This work supports simulations that will advance our ability to understand, predict, and control the structure and electronic properties of functional (nanostructured) interfaces in OPV and DSCs. Employing large-scale, massively parallel quantum mechanical simulations this investigation comprises three research thrusts, each dedicated to one of the three main interface types that are critical for the performance of OPV and DSCs: (i) organic-organic interfaces, (ii) organic-oxide interfaces, and (iii) organic-graphene interfaces. The proposed research will advance the present state-of-the-art in electronic structure methods and advance our ability to develop increased efficiency photovoltaics that support clean and sustainable energy.

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

**Principal Investigator:** David Trebotich, *LBNL*

**Co-Investigators:** Brian Van Straalen (*LBNL*), Anshu Dubey (*LBNL*), Mark Adams (LBNL), Carl Steefel (*LBNL*), Sergi Molins (*LBNL*)

**ALCC allocation: Processor Hours**

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 50,000,000 processor hours

**Site:** Oak Ridge National Laboratory
**Allocation:** 50,000,000 processor hours

**Research Summary:**
Carbon sequestration, the process of removing atmospheric carbon and storing it underground, is a promising technology for mitigating the climate impacts of fossil fuels. A challenge to implementing carbon sequestration is understanding and controlling the geophysics of sequestered carbon. The objective of the DOE Energy Frontier Research Center (EFRC) for Nanoscale Control of Geologic CO2 (NCGC) is to use new investigative tools to build a next-generation understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow and transport in porous rock media, in particular, as applied to geologic sequestration of CO2. To do so, a new generation of experimental imaging tools coupled with simulations and modeling must be developed at the pore scale. To support this effort, this team has developed multiscale, multiphysics simulation tools in the Chombo Framework and have successfully combined Chombo with the complex geochemistry module of CrunchFlow. This project supports further development of the EFRC modeling effort to simulate multiphase, reactive transport processes in realistic pore space obtained from experimental image data. The outcome will be a deepening of our scientific and technical understanding of carbon sequestration and to advance the path towards this promising technology.

**Title:** Delivering Advanced Modeling & Simulation for Nuclear Energy Applications

**Principal Investigator:** John Turner, *ORNL*

**Co-Investigators:** Mark Christon (*LANL*), Tom Downar (*U. of Michigan*), Thomas E. Evans (*ORNL*), Douglas B. Kothe (*ORNL*)

**ALCC allocation: Processor Hours**

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

**Site:** Oak Ridge National Laboratory
**Allocation:** 80,000,000 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.

This allocation supports the continued development of VERA models and methods and insight provided by application of VERA to address 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. 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:** Understanding Helium Plasma Mediated Tungsten Surface Response to better predict Fusion Plasma Facing Component Performance in ITER

**Principal Investigator:** Brian Wirth, *University of Tennessee*

**Co-Investigators:** David Bernholdt (*ORNL*), Jay Jay Billings (*ORNL*), Luis Sandoval (*LANL*), Danny Perez (*LANL*), Blas Uberuaga (*LANL*), Lin Hu (*UMass*), Dimitrios Maroudas (*UMass*), Giridhar Nandipati (*PNNL*), Ken Roche (*PNNL*), Rick Kurtz, (*PNNL*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 66,000,000 processor hours

**Site:** Oak Ridge National Laboratory
**Allocation:** 30,000,000 processor hours

**Research Summary:**

Controlled fusion could provide the world with a near limitless source of clean energy. However, the realization of fusion as a practical energy source requires the ability to build a device that can safely contain the fusion reaction. For magnetically confined fusion plasma reactions, the performance demands on plasma-facing components (PFCs) and structural materials are beyond the capability of current materials. In particular, the plasma surface interactions (PSIs) occurring in the divertor and PFCs pose a critical scientific challenge that limits our ability to achieve electricity production from fusion. The objective of this project is to further advance understanding of the response of tungsten, the proposed ITER divertor, to low energy He plasma exposure. In particular, three tasks are envisioned that investigate helium behavior and gas bubble aggregation kinetics in tungsten, and address whether gas diffusivity is enhanced along grain boundaries. Outcomes of this project will be an improved knowledge of the materials engineering necessary for the success of ITER and critical to this pathway of harnessing fusion energy.

**Title:** Calculation of Neutron Scattering Cross Section of Plutonium and its Compounds

**Principal Investigator:** Gabriel Kotliar, *Rutgers University*

**Co-Investigators:** Kristjan Haul (*Rutgers University*), Viktor Oudovenko (*Rutgers University*), Zhiping Yin (*Rutgers University*), Xiaoyu Deng (*Rutgers University*), Bismayan Chakrabarti (*Rutgers University*)

**ALCC allocation: Processor Hours**
**Site:** Oak Ridge National Laboratory
**Allocation:** 90,000,000 processor hours

**Research Summary:**
Theoretical understanding of the behavior of materials is a great intellectual challenge and will be the key to new technologies. While the nuclear properties of the actinides ( materials containing 5f electrons ) are well understood, their solid state properties are not, and represent a frontier in condensed matter science. Theoretical and computational simulations of actinide materials, is of particular importance given the difficulties and the costs carrying out experiments in this class of systems. This project supports first principles computational studies of scattering cross sections of actinide-based materials which will probe the magnetic excitation spectrum of these systems. The project will couple new theoretical approaches and powerful algorithms for parallel computing with ongoing experimental efforts at the Oak Ridge National Laboratory (ORNL), Los Alamos National Laboratory (LANL) and at the Institute Laue-Langevin (ILL), France which will test and validate the theoretical approach. Outcomes of this project will be a deeper and more advanced theoretical and experimental understanding of actinide materials through the benchmarking of the LDA+DMFT methodology against scattering experiments.

**Title:** Composite Higgs Theory Beyond the Standard Model and the 14 TeV upgrade of the Large Hadron Collider

**Principal Investigator:** Julius Kuti, *UCSD*

**Co-Investigators:** Zoltan Fodor (*University of Wuppertal, Germany*), Kieran Holland (*University of the Pacific*), Santanu Mondal (*Institute for Theoretical Physics, Hungary*), Daniel Nógrádi (*Institute for Theoretical Physics, Hungary*), Chik Him Wong (*UCSD*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory

**Allocation:** 88,700,000 processor hours

**Research Summary:**

The Standard Model is the predominant and most fundamental theory in particle physics for our understanding of the universe at the deepest level. It explains the origin of mass and matter in terms of a specific collection of fundamental particles and their forces. Using the Large Hadron Collider (LHC) of CERN, experiments of large international collaborations test the Standard Model and discover its basic properties from high energy collisions of particles by studying the pieces that result from the collisions. This is how the Higgs particle was recently discovered earning the Nobel prize for its inventors. The LHC will soon undergo a 14 TeV energy upgrade and the new energies available to the LHC14 will extend the search for fundamental new physics Beyond the Standard Model (BSM). The recently discovered Higgs boson could play the role of an important messenger of new BSM physics. Predicted by the Standard Model, the Higgs boson is described as a fundamental particle responsible for the origin of mass in the universe. However, at a deeper level, the Higgs could be a composite of new fundamental particles waiting for discovery in the BSM paradigm. The measured properties of the Higgs as detected by the LHC are not precise enough to validate the Standard Model to the exclusion of alternative composite Higgs models. Based on this team's recent exploratory studies, a promising candidate theory is identified for an alternative composite Higgs mechanism which may be revealed by the LHC14 upgrade. This project supports further investigations in an effort to confirm the preliminary findings with exciting potential for discovery. The outcome of the project will come from the detailed analysis of the theory from simulations that are important for the experimental search of the composite Higgs scenario at the LHC14 looking for evidence of new physics Beyond the Standard Model.

**Title:** Petascale Simulations in Support of CESAR

**Principal Investigator:** Elia Merzari, *ANL*

**Co-Investigators:** Paul Fischer (*ANL*), Andrew Siegel (*ANL*), Vijay Mahadevan (*ANL*), Kord Smith (*MIT*)

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 80,000,000 processor hours

**Research Summary:**

Safer nuclear energy power promises to become a reliable, carbon-free resource capable of meeting our nation's and the world's energy needs. Numerical simulation has been an intrinsic part of nuclear engineering research, design, and licensing of existing and proposed conventional nuclear power plants. Nuclear modeling and simulation tools available today, however, are mostly low dimensional, empirically based, valid for conditions close to the original experiments, and in many cases incremental improvements on decades-old legacy codes. The development, deployment, verification, and validation of higher-fidelity computational capabilities for analyzing, modeling, simulating, and predicting complex thermo-fluid phenomena will help advance nuclear power capabilities by resolving technical, cost, and safety issues. The Center for Exascale Simulation for Advanced Reactors (CESAR), one of the three codesign centers funded by DOE, aims to address these challenges by developing a coupled, next generation nuclear reactor core simulation tool capable of efficient execution on exascale computing platforms. This project supports the mission of CESAR with large petascale level simulations needed to address the limitations of current methods and address the potential scaling to larger machines. The resulting improved state-of-the art simulation code will aid advancements in nuclear engineering and nuclear energy.

**Title:** Nanostructure-enhanced Chemical Reactivity and Detonation in Energetic Materials

**Principal Investigator:** Aidan Thompson, *Sandia National Laboratories*

**Co-Investigators:** Tzu-Ray Shaun (*SNL*), Ryan R. Wixom (*SNL*)

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 80,000,000 processor hours

**Research Summary:**

Understanding the physics and chemistry of detonation in energetic materials is important across many sectors including national security applications, civil engineering (mining and excavation) and in specialized applications such as emergency passenger restraint systems and rocket propulsion. Despite recent advances in our understanding of the initiation of energetic materials, we are yet incapable of accurately predicting the shock-to-detonation transition in real explosives. Using state of the art quantum mechanical dynamics (QMD) methods, we are now equipped with the ability to predict the shock properties of perfect single crystals of energetic materials. However, it is believed that material defects such as entrained solvent, dislocations, porosity, and grain-boundaries play a key role in the onset of shock-induced chemical reactions and the ignition of hot spots. The spatial scales of these phenomena are too small to resolve in continuum models, but are too large for molecular models. A method is needed that bridges between the molecular and continuum scales, but retains the accuracy of quantum methods. The ReaxFF reactive interatomic potential implemented in the LAMMPS parallel molecular dynamics code allows us to bridge these scales by running micron-scale atomistic simulations of void collapse and hotspot formation. The project supports the investigation of nanostructure-enhanced chemical reactivity and detonation in energetic materials and the study of shock energy localization at materials heterogeneities. The outcome of this work will fill a critical gap in energetic materials modeling, enabling predictive models of performance, reliability, and failure ..

**Title:** Turbulent Multiphase Flows for Nuclear Reactor Safety

**Principal Investigator:** Igor A. Bolotnov, *North Carolina State University*

**Co-Investigators:** Michel Rasquin (*ANL*), Hong Yi (*UNC Chapel Hill*), Kenneth E. Jansen (*U. Colorado at Boulder*)

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 76,800,000 processor hours

**Research Summary:**

Most operating nuclear reactors use water to both cool the reactor and transfer the heat from the nuclear fuel to use in electricity generation. Understanding the details of bubbly turbulent flow within a nuclear reactor core is important for design of safe and efficient reactors; however the geometry, high pressure/temperature conditions and boiling nature of the flow in the nuclear reactor core make the analysis of this complex phenomenon a challenge. This project supports simulations of turbulent multiphase flows important for nuclear reactor analysis**.** Direct numerical simulation (DNS) of turbulent bubbly two-phase flows at a leadership computing facility will enable modeling at an unprecedented level of detail and can answer fundamental questions about the interaction between the bubbles and the liquid turbulence. Detailed simulation will enable collecting and obtaining statistical information about the turbulence parameters, such as turbulent kinetic energy and turbulent viscosity. The outcome of this project will be to improve the multiphase computational fluid dynamics (CMFD) closure models in applications to nuclear reactor thermal-hydraulics modeling. This will allow for better safety margin predictions for existing light water reactors and facilitate the development of next generation energy systems.

**Title:** Development of High-Fidelity Multiphase Combustion Models for Large Eddy Simulation of Advanced Engine Systems

**Principal Investigator:** Joseph C. Oefelein, *Sandia National Laboratories*

**Co-Investigators:** Guilhem Lacaze (*SNL*), Rainer Dahms (*SNL*), Christopher Stone (*Computational Science and Engineering LLC*), Roger L. Davis (*UC Davis*), Ramanan Sankaran (*ORNL*)

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

**Research Summary:**

The importance of understanding liquid-fuel injection and multiphase combustion processes in state-of-the-art transportation, propulsion, and power systems (e.g., reciprocating and gas-turbine internal-combustion engines) are widely recognized. Injection of liquid fuels largely determines fuel-air mixture formation, which governs the detailed evolution of chemical kinetics, combustion, and emissions. A lack of accurate models is a major barrier toward the design of advanced engine systems that are clean and highly efficient, and there is a critical need for advanced development in this area. Thus, the objective of this project is to perform fundamental inquiries into the structure and dynamics of turbulent combustion processes that are dominated by high-pressure, high-Reynolds-number, multiphase flows at device relevant conditions. A progressive series of calculations will be performed using the Large Eddy Simulation (LES) technique with two major objectives. The first is to establish a set of high-fidelity computational benchmarks. The second is to establish a scientific foundation for advanced model development. The simulations will be staged by first investigating relevant processes in a well-controlled laboratory scale flame. These results will then be used to accurately scale to liquid-fuel injection and combustion processes present in advanced internal-combustion engines. The simulations will be directly coupled to a set of companion experiments being performed at Sandia National Laboratories, Combustion Research Facility. The results will provide scientific advances required for improved predictive models for combustion design.

**Title:** Molecular Dynamics Studies of Biomass Degradation in Biofuel Production

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

**Co-Investigators:** Rafael C Bernardi (*University of Illinois)*

**ALCC allocation: Processor Hours**

**Site:** Lawrence Berkeley National Laboratory

**Allocation:** 69,000,000 processor hours

**Research Summary:**

Biofuels are a well-known alternative to the largely used fossil-derived fuels, however the competition with food production has established an ethical issue and one of the possible solutions is offered by second-generation biofuels. A critical bottleneck for the production of second-generation biofuel is the depolymerization (breakdown) of plant biomass. The breakdown of plant biomass is not straightforward because plants have evolved complex structural and chemical linkages that are highly resistant to degradation by the microbial enzymes used to release the sugar units for further ethanol production. Advanced computational tools make it feasible to address biomolecular-related problems associated with biofuel production through simulations of the enzymatic systems that act on plant fibers. To address the challenge of producing second-generation biofuels, this project supports a joint computational and experimental approach to study major problems of the second-generation biofuel industry. The outcomes will be a deeper molecular understanding of challenges and solutions for development of second-generation biofuels and advancement along the path towards clean energy.

**Title:** Quark and Glue Structure of the Nucleon with Lattice QCD

**Principal Investigator:** Keh-Fei Liu, *U. Kentucky*

**Co-Investigators:** Terrence Draper (*U. Kentucky*), Andrei Alexandru (*George Washington University*), Frank Lee (*George Washington Unviersity*)

**ALCC allocation: Processor Hours**
**Site:** Oak Ridge National Laboratory
**Allocation:** 68,800,000 processor hours

**Research Summary:**
The Standard Model is an important particle physics theory that describes the universe as a specific collection of fundamental physical and force particles. Quarks are an example of a fundamental matter particle and interact with other quarks through force particles called gluons. Together, the quarks and gluons serve as the building blocks for more commonly known particles such as the proton and neutron (collectively known as nucleons) found in the nuclei of atoms. Studying and understanding the quark-gluon structure of the nucleon and their interactions are therefore of fundamental importance to understanding the building blocks of our universe and life. Quantum Chromodynamics (QCD) is the fundamental theory of quarks and gluons. The aim of this project is to determine how a basic property of a proton, namely its spin, is made up from its constituent quarks and gluons. It will investigate the quark and gluon compositions of the proton spin with a numerical approach called ``Lattice QCD.'' The outcome of this work will be an improved and first-principle-based understanding of the quark-gluon structure of the nucleon which can be compared with experiments being conducted in high energy and nuclear physics laboratories around the world.

**Title:** Molecular Simulation in Bioenergy

**Principal Investigator:** Jeremy Smith, *Oak Ridge National Laboratory*

**Co-Investigators:** Xiaolin Cheng (*ORNL*), Loukas Petridis (*ORNL*)

**ALCC allocation: Processor Hours**
**Site:** Oak Ridge National Laboratory
**Allocation:** 59,000,000 processor hours

**Research Summary:**

Biofuels offer a promising clean-energy alternative to many fossil fuel types. One important challenge to utilizing biofuels is developing methods for efficient production of biofuels from the plant source. A molecular-level understanding of structure and function is fundamental to research into improving the efficiency of biofuel production. Lignocellulosic biomass is a complex plant material that presents a particular challenge to biofuel production. This project supports simulations that will help obtain a detailed knowledge of the fundamental molecular organization, interactions, mechanics and associations of bulk lignocellulosic biomass and its interaction with enzymes that catalyze the conversion of biomass into fermentable sugars. This work forms an integral part of a larger effort comprising the Bioenergy Science Center (BESC) and the ORNL Biofuels Science Focus Area (SFA), aimed at integrating experimental and leadership-class computation to synergistically derive information on lignocellulosic degradation by enzymes at an unprecedented level of detail and advance our ability to efficiently produce biofuels.

**Title:** Influence of Morhphology on Proton Transport in Proton Exchange Membranes

**Principal Investigator:** Gregory Voth, *U. Chicago / Argonne National Laboratory*

**Co-Investigators:** Christopher Knight (*ANL*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory

**Allocation:** 57,600,000 processor hours

**Research Summary:**

Powering society with alternative technologies to fossil fuel combustion has been increasingly recognized as a national security priority. Included in alternative technologies are electrochemical energy-conversion devices, such as fuel cell. The successful development of low-cost, high-performance electrochemical devices would have an important impact in the clean energy market. To date, the rate-limiting step in the optimization and design of new materials for such systems has been the use of intuition based “guess and check” strategies. The efficiency of this strategy can be significantly improved with the incorporation of a detailed fundamental understanding of the associated transport processes based on the results of combining experimental characterization and molecular modeling. The project utilizes a combination of novel molecular simulation algorithms developed by this team to improve the understanding of fundamental processes that govern charge transport in polymer electrolyte membranes commonly used in fuel cells. The ability to satisfy all criteria for realistic calculations on these important systems will be accomplished by the coupling of accurate reactive dynamics models, a highly efficient simulation software package and parallelization strategies specifically tailored to multistate simulations. The outcome of the project will be a significant step forward on answering fundamental questions regarding proton transport in fuel cell membranes and stimulating the synergy of theoretical and experimental characterizations of these important systems.

**Title:** Quantum Computational Science

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

**Co-Investigators:** Federico Spedalieri (*University of Southern California*), Rosa Di Felice (*University of Southern California*), Travis S. Humble (*ORNL*), Bobby Sumpter (*ORNL*), Daniel Lidar (*University of Southern California*), Tameem Albash (*University of Southern California*), Matthias Troyer (*ETH Zurich, Switzerland*), Greg Tallant (*Lockheed Martin*)

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

**Research Summary:**

With recent theoretical and experimental advances in the field of Quantum Computing, quantum computers are emerging as extremely valuable tools for scientific research. However, since quantum computers are scarce, one can only hope to gain insight into their capabilities and potential, as well as their limitations, via simulations or other approximation schemes performed on classical computers. Such simulations are usually very resource demanding because the classical description of quantum systems grows exponentially with system size. This project is twofold and supports (i) testing of 'adiabatic quantum computing', a proposed paradigm for quantum computation, specifically, the D-Wave Two quantum annealer, and (ii) molecular dynamic and electronic structure calculations of important biological and chemical target systems for future exploration on quantum computers. The outcomes of this project will support testing the limits of near term Quantum Computing devices and represent important steps along the path to realizing the potential of quantum computing.

**Title:** Simulation of Large Hadron Collider Events Using Leadership Computing

**Principal Investigator:** Thomas LeCompte, *Argonne National Laboratory*

**Co-Investigators:** Doug Benjamin (*Duke University*), Richard Mount (*SLAC National Laboratory*), J. Taylor Childers (*ANL*), Thomas D. Uram (*ANL*), Venkat Vishwanath (*ANL*)

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 50,000,000 processor hours

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 2,000,000 processor hours

**Research Summary:**

The Large Hadron Collider (LHC) is one of the largest and most complex experimental facilities ever built, with six experiments exploring the behavior of matter, energy, space and time at the shortest distance scales ever probed. The LHC accelerates counter-circulating beams of protons to very high energies which then collide in the center of building-sized particle detectors like ATLAS. These detectors – each operated by a worldwide collaboration of 3000 scientists (about 20% from the US) – measure the positions, momenta and properties of the particles produced in these collisions, and the scientific teams use these measurements to infer what happened in each collision, *e.g*. the production of a Higgs boson. The computational requirements for such experiments are extremely large and growing, and we can imagine a time in the near future where the science is limited not by the number of events that the LHC can produce but instead the number of events our Grid based computers can simulate. Additionally, even today there are events that are too complex to simulate on the Grid at the scale needed by the experiments' analysis teams. This allocation supports an effort to address this challenge by running a small but noticeable fraction of ATLAS simulation events on DOE supercomputers, particularly those that are difficult to produce any other way. The outcomes will support advances in high energy physics and shed light on a possible path forward for analyzing future LHC data.

**Title:** Advanced Simulation of HFIR for LEU Conversion

**Principal Investigator:** Gregory Davidson, *ORNL*

**Co-Investigators:** Thomas M. Evans (*ORNL*), Tara Pandya (*ORNL*), Seth Johnson (*ORNL*)

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

**Research Summary:**

An important program within the NNSA Global Threat Reduction Initiative aims to convert research and test reactors that use high enriched uranium (HEU) to low enriched uranium (LEU) as a means to reduce the availability of weapons-usable material. The program has converted all of the U.S. domestic research reactors that can be successfully converted to LEU using existing qualified fuels. However, there are six high-performance research reactors (HPRRs) for which conversion has been delayed due to the significant changes to the fuel required if these reactors are to become LEU reactors. The need for the fuel modification creates two primary challenges. The first is the development and qualification of fabrication approaches for the fuel and ensuring that the fuel can meet all materials performance requirements. The second is the analysis that is necessary to (a) support design and/or operational changes that would result in a minimal impact on reactor performance, and (b) to support the necessary safety basis for conversion to LEU. This project supports advanced modeling and simulation (M&S) to improve prediction of operational performance, ensuring safe operation of the reactor; to reduce requirements on fuel fabrication and performance through better prediction of localized power peaking and temperatures; and to support the development of the high density fuels. The outcomes will be important steps towards fuel design for LEU reactors and meeting the goals of the NNSA Global Threat Reduction Initiative.

**Title:** Gyrokinetic Simulation of Energetic Particle Turbulence and Transport.

**Principal Investigator:** Zhihong Lin, *U.C. Irvine*

**Co-Investigators:** Ronald Waltz (*General Atomics*), Donald Spong (*ORNL*)

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

**Research Summary:**

Fusion is a promising technology for near limitless clean energy. The International Thermonuclear Experimental Reactor (ITER) is a multi-national collaboration to build a test nuclear fusion reactor. Success of ITER would represent a large step towards the realization of fusion as a future energy source. Although under construction, ITER still must address many scientific and technological challenges. One example is the successful confinement of the fusion products—energetic particles in the burning plasma. The performance of ITER depends on the confinement of and self-heating by energetic particles within the plasma. Many challenges make accurately predicting confinement properties of energetic particles difficult. Examples include self-consistent incorporation of kinetic effects and nonlinear interactions of many plasma waves (specifically 'shear Alfven wave turbulence'). This project supports simulations that will comprehensively assess the confinement properties of the energetic particles in the ITER experiment. The project will use state-of-the-art gyrokinetic turbulence simulations developed to address the challenges of modeling energetic particle confinement in burning plasma. Outcomes will be an improved predictive understanding of plasma confinement in ITER that will further the chance of ITER's success and represent an important step towards harnessing fusion energy.

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

**Principal Investigator:** Ron Brightwell, *SNL*

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

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 5,000,000 processor hours

**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 5,000,000 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; dramatically improve power efficiency, improve resilience in the presence of increasing faults, enable efficient data movement across deepening memory hierarchies and new storage technologies, and 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 OS 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 enables application composition through lightweight virtualization. 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. While much of the exploration and development of the Hobbes software environment can be done at small scale, evaluating the scalability of OS/R interfaces and mechanisms at large scale is crucial. This project supports large scale testing and evaluation of OS/R implementation techniques to improve OS/R for future high performance computing machines.

**Title:** Uncertainty Quantification in Coal Gasifier Simulations For Clean Energy Technology Development and Production

**Principal Investigator:** Aytekin Gel, *ALPEMI Consulting LLC / NETL*

**Co-Investigators:** Mehrdad Shahnam (U.S. Department of Energy National Energy Technology Laboratory), Arun Subramaniyan (*GE Global Research Center*), Jordan Musser (U.S. Department of Energy National Energy Technology Laboratory)

**ALCC allocation: Processor Hours**

**Site:** Lawrence Berkeley National Laboratory

**Allocation:** 37,500,000 processor hours

**Research Summary:**

Advanced power generation technologies such as Integrated Gasification Combined Cycle (IGCC) plants can potentially reduce the adverse impact of coal utilization on the environment. In an IGCC power plant, a gasifier converts coal into synthesis gas (syngas), which after the removal of impurities and pollutants, is used in a gas turbine to generate electricity.

Advanced computational modeling and simulation capabilities promise to significantly reduce the time and cost of the development and deployment of these next generation clean coal-based technologies. However, the credibility of these simulations must be established with the aid of uncertainty quantification methods to ensure their usefulness within the design processes. For this purpose, non-intrusive Bayesian uncertainty quantification methods will be used to efficiently propagate input uncertainties through deterministic computational fluid dynamics models and quantify model uncertainty. Extensive coal gasifier experimental data from a bench-scale fluidized bed gasifier will be used to quantify model discrepancy as well as validate simulation results. This type rigorous model discrepancy assessment is crucial in making simulation a more trusted support tool in the deployment of advanced clean coal-based power generation technologies.

**Title:** Amplitude Modulation of Wind Turbine Noise

**Principal Investigator:** Sanjiva Lele, *Stanford University*

**Co-Investigators:** Joseph Kocheemoolayil (*Stanford U.*), Giridhar Jothiprasad (*GE*), Lawrence Cheung (*GE*), Ramesh Balakrishnan (*ANL*)

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 36,500,000 processor hours

**Research Summary:**

Deployment of large wind turbines in large scale wind farm projects as a renewable energy technology helps address concerns over greenhouse gas emissions and reliance on hydrocarbon based energy sources. However as large-scale wind energy projects are developed significant concerns about the noise from wind turbines have arisen and in some cases become a barrier to further development of wind resources. There is particular concern over an intermittent form of intense wind turbine noise, described as 'intermittent thumping'. However, the aerodynamic mechanisms which create these intense noises, presently categorized as other amplitude modulation (OAM), are poorly understood. This allocation supports investigations that will deepen the scientific understanding of intense noise emission associated with OAM using physics-based simulations designed to capture the flow-phenomenon responsible for its generation. The outcome will be a greater physical understanding of wind turbine noise that will be important for improved wind turbine design, implementation, and clean energy.

**Title:** Prediction and design of energy materials by petascale evolutionary algorithm simulations

**Principal Investigator:** Giancarlo Trimarchi, *Northwestern University*

**Co-Investigators:** Alex Zunger, (*U. Colorado*), Xiuwen Zhang (*U. Colorado*), Arthur J. Freeman (*Northwestern University*)

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 30,000,000 processor hours

**Research Summary:**

The materials properties that enable a range of energy related technologies, such as PV absorbers, transparent conductors, and photo-catalysis, to mention just a few, tend to "live" in materials with specific compositions and crystal structures—and no others. The search for optimal energy materials should not be limited to the databases of currently known materials, but it should be extended to the large number of element combinations that define chemically possible compounds that are missing from such compilations. In order to predict the properties of such materials missing from the current databases, one first needs to predict whether they are thermodynamically stable, i.e., can be synthesized, and in what crystal structure. The problem of predicting the crystal structure of a material starting from the elemental constituents and without any bias is one of the most challenging problems in condensed matter physics. An important recent advance in this field has been the development of evolutionary algorithms coupled with density functional theory to predict the crystal structure of a solid without assumptions. This project supports the development, testing, and application of improved crystal structure prediction methods based on state-of-the-art *ab initio* electronic structure techniques and evolutionary algorithms to simultaneously search for materials with stable structures and target properties. The objective is to make these optimization methods scale to larger crystal structures than it is now possible and to apply them to search for materials that meet the design principles of desired functionalities without constraints and going beyond the databases of known compounds. In addition to these computational advances, in this work we will predict the stable structures and energy-related properties of many new solids that might include numerous materials with thus far unsuspected and exciting functionalities for energy applications.

**Title:** Gyrokinetic Simulations of the Effect of Electron Heating on Particle and Electron Thermal Energy Transport in Magnetic Fusion Plasmas

**Principal Investigator:** D.R. Ernst, *MIT*

**Co-Investigators:** W. Guttenfelder (*Princeton University Plasma Physics Laboratory*), A. Dimits (*Lawrence Livermore National Laboratory*)

**ALCC allocation: Processor Hours**

**Site:** Lawrence Berkeley National Laboratory

**Allocation:** 30,000,000 processor hours

**Research Summary:**

Harnessing fusion energy would enable a near limitless clean energy supply for the world. The International Thermonuclear Experimental Reactor is an international research effort to build an experimental fusion reactor. The reactor will use magnetically confined plasma as an approach to produce controlled thermonuclear fusion energy. Understanding the physics of the fusion plasma, and the turbulence which causes loss of particles and energy, is key to the success of ITER. One type of turbulence, 'trapped electron mode (TEM) turbulence', is of particular importance in self-heated fusion plasmas where mainly the electrons are heated. The role of TEM turbulence can be tested on the two major U.S. tokamak facilities, Alcator C-Mod and DIII-D. We have conducted TEM experiments on Alcator C-Mod, and on DIII-D as part of the National Fusion Science Campaign using dominantly electron heating. The experiments feature a suite of local fluctuation measurements and density profiles measured with high resolution. This project supports comparison of these experimental results with computer simulations in unprecedented detail. This work will feature high-risk simulations with very high resolution, directly comparing gyrokinetic simulations with fluctuation measurements that appear to provide the first direct observation of individual density gradient driven trapped electron modes. The outcome will support our physical understanding of magnetically confined plasmas and aid ITER as an important step in realizing thermonuclear controlled fusion.

**Title:** Laser-driven relativistic electron beam filamentation in solids

**Principal Investigator:** Andreas Kemp, *Lawrence Livermore National Laboratory*

**Co-Investigators:** Frederic Perez (*LLNL*), Bruce Cohen (*LLNL*), Laurent Divol (*LLNL*), Pravesh Patel (*LLNL*), Yasuhiko Sentoku (*UNR*)

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

**Research Summary:**

Modern laser beam facilities commonly create plasmas of high energy density by accelerating electrons in the laser focus to relativistic energies; they travel near the speed of light and can no longer be described by classical Newtonian mechanics. Studying these many-body relativistic systems is a grand challenge. It relates High Energy Density Laboratory Physics (HEDLP) –the physics of matter at ultra-high pressure and temperature—to fundamental astrophysical problems like gamma-ray bursts and the origin of cosmic rays, and it has applications ranging from fusion energy to controlled amplification of desirable radiation or particle beams. One specific example application is short-pulse laser experiments planned at the world's most intense x-ray laser source at the 'Matter in Extreme Conditions' instrument at the Stanford Linear Accelerator Center (MEC/SLAC). This project supports relativistic collisional-kinetic simulations of laser-plasma interactions for conditions found at the MEC/SLAC laser facility. The outcome of the project will be a deeper understanding of laser plasma physics, improved methods of simulations, and physics essential to interpretation of short pulse laser experiments planned at MEC/SLAC and similar lasers.

**Title:** Computational Analysis of Complex Proteogenomics Data for Characterization of Terrestrial Carbon Turnover by Soil Microbial Communities

**Principal Investigator:** Chongle Pan, *ORNL*

**Co-Investigators:** Jillian Banfield (U.C. Berkeley)

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 25,000,000 processor hours

**Research Summary:**

Understanding the carbon cycle is of fundamental importance to accurate prediction of future climate change. Grasslands account for ~34% of the global terrestrial carbon reservoir and the majority of fixed carbon in grasslands is stored in soil. Thus to build accurate carbon cycling models, it is critical to understand the carbon cycling in grassland soils. However, much organic carbon in soil is cycled by complex, poorly defined communities through unknown and interconnected networks. The response of these massive reservoirs of organic carbon stored in grassland soils to coming climate changes is unknown because we do not understand how soil microbial communities respond to altered surface vegetation, soil temperature and precipitation. Proteogenomics can be used to elucidate the functionality of the soil microbial communities on a molecular resolution. Proteogenomics combines experimental methods and computational analyses to collect, characterize, and study the entire genome of an organism and the resulting proteins produced by that organism's genome. Thanks to the development of next-generation sequencing and high-resolution mass spectrometry, proteogenomics has become a key data-driven technology for characterization of microbial communities in natural environments. This project supports the scaling up of proteogenomics analyses to extremely complex soil communities in a model grassland ecosystem located in the Angelo reserve. The research aims to determine which organisms, and by what processes, organic carbon is metabolized in deeper soil and the extent to which these are resilient to changes in climate associated with altered rainfall inputs. Outcomes of this proposal will be to broaden the use of leadership computing resources to the proteogenomics community generally and to specifically advance our understanding of terrestrial carbon turnover by microbial communities.

**Title:** High Fidelity Simulations of Combustion Approaches with Increased Efficiency and Reduced Emissions

**Principal Investigator:** Peter Cocks, *United Technologies Research Center*

**Co-Investigators:** Marios C. Soteriou (*UTRC*)

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

**Research Summary:**
Gas turbine combustors are commonly employed as the power source in a wide range of applications, including aircraft, tanks, and ground based power generation. Reducing the emissions and improving the efficiency of gas turbine combustors would therefore have an important impact on environmental health and energy efficiency. Due to the high maturity level of current gas turbine combustors, such goals can only be achieved with a step change in technology. Two promising approaches to combustion for reducing emissions and improving energy efficiency of gas turbine combustors are 'lean combustion' and 'constant volume combustion', respectively. The goal of lean combustion is to reduce peak temperatures inside the combustor, resulting in reduced NOx emissions. For constant volume combustion, the goal is to alter the traditional gas turbine combustor technology which operates using a constant pressure combustion thermodynamic cycle. The constant volume combustion thermodynamic cycle is superior to that for constant pressure, mainly through a reduction in wasted energy (entropy reduction), and this benefit can be used to reduce the specific fuel consumption of gas turbine technology. Although constant volume and lean combustion have significant advantages, the physical processes occurring in combustor concepts leveraging these approaches is complex and not yet well understood. This project supports computational fluid dynamics simulations for an in depth analysis of the physical processes occurring in lean combustion and constant volume combustion. Outcomes will be important scientific insights that will be used for design and implementation of gas turbines with reduced emissions and increased energy efficiency.

**Title:** Multi-scale Water Cycle Processes in Climate Change: Sensitivity to Modeling Frameworks

**Principal Investigator:** Ruby Leung, *Pacific Northwest National Laboratory*

**ALCC allocation: Processor Hours**
**Site:** Oak Ridge National Laboratory
**Allocation:** 18,000,000 processor hours

**Research Summary:**

Climate simulations, particularly the water cycle by global climate models, are sensitive to various sources of uncertainty including representations of physical processes such as clouds, spatial resolutions, and dynamical frameworks. These uncertainties pose challenges for robust simulations of climate and projection of its future change. Among the uncertainties discussed, the impacts of model resolution may be most wide ranging. To address this critical issue, this project supports a series of climate simulations using the Community Atmosphere Model (CAM5) in various configurations focusing on water cycle processes such as cloud, precipitation, and runoff. The proposed simulations are designed to highlight the integral role of multi-scale water cycle processes in future climate change and uncertainties related to combined effects of physics parameterizations, model resolution, and dynamical frameworks on climate change projections. Understanding the sensitivity of climate simulations to various factors will contribute to the *overarching goal of characterizing uncertainties in climate change projections*.

**Title:** Simulating cyclic variability in dilute internal combustion engine operation

**Principal Investigator:** Charles Finney, *ORNL*

**Co-Investigators:** Sreekanth Pannala (*ORNL*), Miroslav K. Stoyanov (*ORNL*), Brad VanDerWege (*Ford Motor Company*), Daniel Lee (*Convergent Science, Inc*), Eric Pomraning (*Convergent Science, Inc*), Keith Richards (*Convergent Science, Inc*), P. Kelly Senecal (*Convergent Science, Inc*)

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 17,500,000 processor hours

**Research Summary:**

Gasoline fueled internal combustion engines serve as the power source for passenger and light-duty vehicles. Improving the fuel economy and emissions of gasoline combustion engines would have an important impact on energy efficiency and clean energy goals. Some strategies to reduce emissions include running the engine highly dilute, with excess air or with recirculated exhaust gases as part of the combustion charge. However, increased dilution leads to increased combustion instability resulting in reduced fuel-economy benefits. This limits the practical range of operation in real-world applications. This project supports computational high-dimensional fluid dynamics simulations to explore the nature and causes of cyclic variability under highly dilute engine cycles. Through methods development in parallelization and intelligent parameter space sampling, this methodology aims to enhance the utility of complex CFD simulations for studying the dynamics of cycle-to-cycle variations in unstable dilute combustion operation.

**Title:** Multi-hole injector optimization for spark-ignited direct-injection gasoline engines

**Principal Investigator:** Tang-Wei Kuo, *General Motors (GM)*

**Co-Investigators:** Ronald Grover (*GM*), Sreekanth Pannala (*ORNL*), Wael Elwasif (*ORNL*)

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 15,000,000 processor hours

**Research Summary:**

Gasoline engines are ubiquitous and designs that improve energy efficiency of gasoline engines can have a significant impact on energy consumption. For combustion to occur in a gasoline engine, the engine must create an air and fuel mixture which can then be ignited by a spark plug inside the combustion chamber. The correct dispersion of fuel in the air is critical to optimum engine performance. In most current automotive gasoline engines, the engine premixes the air and fuel before entry into the combustion chambers. However, greater energy efficiency could be achieved through direct injection of fuel into the combustion chamber hence 'spark-ignited direct injection' (SIDI). Realizing the optimum energy gains from a SIDI engine is a technical challenge. Recently, the most popular SIDI gasoline injectors have been multi-hole type. Multi-hole sprays offer the flexibility of manufacturing the nozzle holes at various orientations to engineer a variety of spray patterns. This flexibility offers a high degree of freedom for design and engine manufacturers need to balance the cost of hardware testing with turn-around time and practicality for mass production. Consequently, detailed analytical tools, such as computational fluid dynamics, become attractive to reduce the number of probable injector concepts for a given combustion system. This project supports the simulations of multi-hole injector designs for SIDI engines. The outcome will be a deeper scientific understanding of spray-injection, a technical challenge in many fields, and advances in engine design and technology to improve automotive energy efficiency.

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

**Principal Investigator:** Christine Hrenya, *U. Colorado*

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

**ALCC allocation: Processor Hours**
**Site:** Oak Ridge National Laboratory
**Allocation:** 15,000,000 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:** Understanding secondary motions and their impact in modeling turbulent flows

**Principal Investigator:** Hassan Nagib, *Illinois Institute of Technology*

**ALCC allocation: Processor Hours**
**Site:** Argonne National Laboratory
**Allocation:** 11,000,000 processor hours

**Research Summary:**
Wall-bounded turbulence is a fundamental scientific topic important to a broad range of industrial, environmental, or any other application that involves bounded turbulence. This project supports simulations that will provide a deeper understanding of wall-bounded turbulence and builds upon important and successful work from a previous 2013 ALCC award. The allocation will advance two main goals: first, this study will provide a deeper fundamental understanding of wall-bounded turbulence, and of the mechanisms responsible for three-dimensional effects in industrial flows. Second, the data collected in this project will help to develop more accurate turbulence models, since the currently available industrial codes still fail to accurately predict three-dimensional flows with secondary motions. The project will fundamentally advance our understanding of comparisons between experimental and computational representations of canonical flows, including further insight on the largest volume of direct numerical simulation data in the literature; i.e., channel flows. The outcome of the project will be a greater fundamental understanding of duct-flows and support future optimization of the wide array of sectors that encounter with wall bounded turbulent flows.

**Title:** Energy coupling in membrane protein function: Mechanisms of Na+-coupled transporters and effects of their environment

**Principal Investigator:** Harel Weinstein, *Cornell University*

**Co-Investigators:** Aurelio Galli (*Vanderbilt University*), Jonathan Javitch (*Columbia*), Ulrik Gether (*University of Copenhagen, Denmark*), George Khelashvili and Scott Blanchard (*Weill Cornell Medical College*)

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

**Research Summary:**
Cells, the fundamental building blocks of life, must engage in all the tasks required for survival such as building cell membranes, protecting and replicating DNA, extracting energy from food, and communication with the external world. All of these tasks are accomplished by the cell on the nanoscale through the use of molecular machines. Understanding the functionality of these molecular machines at a fundamental and atomic level represents one of the ultimate challenges of modern-day life sciences. To advance this effort, this project uses atomistic molecular dynamics to study the fundamental mechanisms in Neurotransmitter Sodium:Symporters (NSS), a type of molecular machine that lives in the membrane of cells and is responsible for moving vital substrates between the cell's external and internal environments. These substrates include neurotransmitters, small molecules used for communication between neurons in mammals, nutrients in bacterial cells, and many exogenous agents such as needed metals, but also natural and synthetic psychoactive agents, abused drugs, and environmental toxicants. The movement of substrates through these molecular machines is driven by energy generated and distributed within the biological systems. This allocation supports the development of detailed analyses of dynamic properties and energetics of the NSS molecules under normal physiological conditions in the cell, and when they are impacted by various interactions in their environments. Outcomes of this project will contribute to significant new understanding of many aspects of the structure, function, spatial organization, and external modulation of these important molecular machines and the energy that drives them, in naturally occurring and synthetically engineered environments. This will advance our understanding of natural molecular machinery for future bioengineering efforts.

**Title:** Controlling conductivity in high-Al content AlGaN by understanding defect formation energies via DFT

**Principal Investigator:** Benjamin Gaddy, *NCSU*

**Co-Investigators:** Douglas L. Irving (*NCSU*), Ramon Collazo, (*NCSU*), Zlatko Sitar (*NCSU*), Baxter Moody (*HexaTech*)

**ALCC allocation: Processor Hours**
**Site:** Lawrence Berkeley National Laboratory
**Allocation:** 7,000,000 processor hours

**Research Summary:**
Creating electronic devices based on aluminum gallium nitride (AlGaN), a semiconductor material, will enable higher power densities and lower energy losses. However, successfully 'doping' AlGaN with high aluminum concentrations has remained a challenge. Doping is a process of adding impurities to materials in order to control and adjust their electrical properties. Interestingly, dopants typically used for AlGaN with low concentrations of aluminum (Si and O) are known to create unacceptably low conductivities for AlGaN with high concentrations of aluminum. The transition has been shown to occur for Al concentrations above about 70%. Understanding the reason for the transition could enable the realization of superior AlGaN electronic devices, yet the origin of this transition is still unknown. Recent studies suggest the origin for the transition may reside in small structural defects introduced by the doping agents. This project supports electronic structure theory calculations that will model defect formation energies of a host of relevant native and impurity defects in AlGaN alloys. A database will be produced containing various structural properties, electronic properties, and formation energies as a function of various impurity defects. The outcome of this work will enable understanding of the transition, provide insights into strategies for successful doping of AlGaN, and represent an important step forward in producing more effective electronic materials.

**Title:** Application of munerical time-reversal mirror for the construction of continental scale tomographic model of the upper mantle based on full waveform seismic inversion

**Principal Investigator:** Barbara Romanowicz, *U.C. Berkley*

**Co-Investigators:** Thomas Bodin (*U.C. Berkeley*), Marco Calo (*U.C. Berkeley*), Scott French (*U.C. Berkeley*), Zhao Zheng (*U.C. Berkeley*), Yder Masson (*Institute de Physique du Globe de Paris , France*)

**ALCC allocation: Processor Hours**

**Site:** Lawrence Berkeley National Laboratory

**Allocation:** 6,000,000 processor hours

**Research Summary:**

When an earthquake or an underground explosion occurs, the seismic waves that are generated propagate through the Earth, illuminating its three dimensional (3D) structure, while also carrying the signature of the source. The seismic wavefield generated by many events and recorded at many stations around the world can be used to image the structure using tomographic approaches. This is a rapidly developing field, which provides the most important constraints to further our understanding of our planet's present day and past dynamics, and the driving mechanisms for plate tectonics. Outcomes of such research are valuable to many fields including nuclear monitoring, environmental monitoring, geophysical prospecting, and prediction of seismic events. This project supports development of a three-dimensional seismic tomographic model of shear velocity in the upper mantle for the North American continent, using numerical waveform modeling. The approach will use the first-ever SEM-based continental-scale inversion that includes global constraints using a time-reversal mirror, which represents a new frontier in seismological research

**Title:** Large Scale Turbulent Clean Coal Combustion

**Principal Investigator:** Martin Berzins, *University of Utah*

**Co-Investigators:** Jeremy Thornock, Todd Harman, John Schmidt, James Sutherland, (University of Utah).

**ALCC allocation: Processor Hours**

**Site:** Argonne National Laboratory
**Allocation:** 10,000,000 processor hours

**Site:** Oak Ridge National Laboratory
**Allocation:** 30,000,000 processor hours

**Research Summary:**

Domestic coal offers the potential for reaching secure inexpensive sources of fuel for at least many hundreds of years but only if new technologies are used to extract and utilize this energy resource in ways that protect the environment. Breakthroughs in clean energy can provide benefits to the economy, security, environment, and jobs. Energy research and advancements will be revolutionized by simulation-based science. Exascale simulation science offers the potential for not only discovering new technologies but for more rapidly implementing new inventions at a scale sufficient to displace or augment existing energy options. This work supports code development for enabling full machine utilization (CPU and GPUI) of the largest possible Large Eddy Simulations for oxy-goal boiler modeling. The outcome of this project will be an important step towards enabling petascale simulated guided design for next generation oxy-coal boilers for clean energy.

**Title:** Supersonic Compression & Engine Technology: Time-Varying Phenomena & Geometric Optimization

**Principal Investigator:** Ravi Srinivasan, *Ramgen Power Systems, LLC.*

**Co-Investigators:** Logan Sailer (Ramgen), Alain Demeulenaere (Numeca), David Gutzwiller (Numeca), Mathieu Gontier (Numeca).

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 16,600,000 processor hours

**Research Summary:**

One of the most pressing scientific challenges facing the United States and the world is reducing greenhouse gas emissions. Compounding that challenge is the fact that power plants burning fossil fuels account for more than 40% of the world's energy-related CO2 emissions and will continue to dominate the supply of electricity until the middle of the century. There is an urgent need for cost-effective methods to capture and store their carbon emissions. The principal barrier to widespread application of Carbon Capture and Sequestration (CCS) is its cost. Once the CO2 is captured, compressing it to the required 100 atmospheres represents approximately 33% of the total cost of CCS. This project supports the development of supersonic compression technology to reduce the cost of CO2 compression for CCS by developing efficient, very high-pressure ratio compressors. Utilization of OLCF's Titan supercomputing system can dramatically accelerate the design time-line and performance of high-pressure ratio supersonic compressors. The project will result in more cost-effective compressions techniques and a more detailed understanding of supersonic turbomachinery flow physics.

**Title:** Hypernuclei and Charmed Nuclei

**Principal Investigator:** Martin J. Savage, *Institute for Nuclear Theory*

**Co-Investigators:** Silas R. Beane (*U. Wash*), William Detmold (*MIT*), Kostas Orginos (*College of William and Mary*)

**ALCC allocation: Processor Hours**

**Site:** Oak Ridge National Laboratory

**Allocation:** 65,100,000 processor hours

**Research Summary:**

Whether it be radioactive uranium or a stable neon gas, across the periodic table all atomic nuclei are composed of two types of quarks; “up” and “down”. Under the extreme conditions made possible at accelerators, exotic nuclei containing “strange” quarks, called Hypernuclei, are created and studied, and those containing “charm” quarks, called Charmed Nuclei, have been conjectured to exist. These exciting rare nuclei provide key insights into the workings and behavior of fundamental particles in our universe and are now the focus of a new generation of experiments. These experiments aim to measure the basic properties of Hypernuclei and Charmed Nuclei with relatively high precision. However, these special nuclei are exceptionally rare and extremely challenging to produce. Simulations are pivotal in examining theory and guiding experiment. This project supports high performance computational simulations of the Hypernuclei and Charmed Nuclei that are expected to be produced in upcoming experiments. The results of this work will support, and provide new directions for the US experimental programs at the Brookhaven National Laboratory and the Thomas Jefferson National Accelerator Facility, and experiments in Japan and Europe.