2010 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: "A Scalable, Efficient, and Accurate Community Ice Sheet Model (SEACISM)"

Principal Investigator: Katherine Evans, Oak Ridge National Laboratory
Co-Investigators: Patrick Worley, Oak Ridge National Laboratory,
James (Trey) White, Oak Ridge National Laboratory,
Andy Salinger, Sandia National Laboratories,
William Lipscomb, Los Alamos National Laboratory

ALCC allocation:

Site: Argonne National Laboratory
Allocation: 1,000,000 processor hours

Site: Oak Ridge National Laboratory
Allocation: 5,000,000 processor hours

Research Summary:
Sea level rise associated with reductions in ice sheet volume is one of the most poorly constrained yet globally important consequences of climate change. The importance of ice sheets was underscored in the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (AR4), which provided neither a best estimate nor an upper bound for 21st century sea-level rise. This was largely due to uncertainties concerning the dynamical response of ice sheets to climate change. Recent observations have identified that ice sheets can respond to climate change on annual to decadal time scales and that the Greenland and West Antarctic ice sheets are losing mass at an increasing rate. Further, observations confirm that current mass loss from Greenland and Antarctic ice sheets is dominated by acceleration and thinning of large outlet glaciers and ice streams; however, sea-level projections referenced in the AR4 are based largely on models that do not capture these dynamics adequately and thus underestimate the risk of rapid sea-level rise. In the climate research community, significant efforts are underway to improve ice sheet models for use in Earth system models and instantiate a model predictive capability. The time scale to develop ice sheet models with next generation computing capabilities for scientific research and policy advising is very short, and these improvements require state-of-the-art solver technology and utilization of leadership class computing platforms. This project will develop a scalable, efficient, and accurate ice sheet model within the required time frame.

Title: "Aerodynamics Exploration for Advanced Aero-Propulsion Technologies"

Principal Investigator: Jixian Yao, GE Global Research
Co-Investigators: Graham Holmes, GE Global Research

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 4,500,000 processor hours

Research Summary:
This project will explore the promising aerodynamic technologies that lead to the successful development of advanced aero-engine propulsors. Advanced propulsor design employs a low-pressure-ratio fan and its driving component, a light-weight, high-output, low-pressure turbine. These propulsors employ higher bypass ratio, low-pressure ratio fan designs for improved fuel burn. Lower fan pressure ratios lead to increased propulsive efficiency, enable thermodynamic cycle changes for improved fuel efficiency, and allow significant noise reduction to be achieved. However, as the fan pressure ratio and fan speed are reduced, the fan design becomes more sensitive to inlet flow distortion and installation stagnation pressure losses. This project will perform rigorous investigation of the underlying mechanism and necessary technologies to reduce inlet distortion sensitivity and stability issues in low-pressure (LP) ratio aero-engine fan systems. Being able to understand and predict the unsteady transitional flow in LP turbines is essential in developing airfoils with increased lift and increased stage loading that retain the already high levels of efficiency. The three-dimensional design of LP turbine airfoils also holds tremendous promise for achieving improved performance.

Title: "Materials Design From First Principles Calculations"

Principal Investigator: Larry Curtiss, Argonne National Laboratory
Co-Investigators: Stephan Gray, Argonne National Laboratory,
Jeffrey Greeley, Argonne National Laboratory,
Jeff Hammond, Argonne National Laboratory,
Nichols Romero, Argonne National Laboratory,
Peter Zapol, Argonne National Laboratory

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

Research Summary:
The design and discovery of new materials are crucial to our energy future. Massively parallel quantum chemical calculations will play a key role in the design of breakthrough materials to help make the advances needed. This project will provide the fundamental understanding and predictions needed to design new materials for catalysis and electrical energy storage. The project will use new electronic structure codes that are just becoming available for massively parallel computer clusters, in combination with new concepts in materials design based on descriptors for large scale screening and synergies with world-leading experimental groups in catalysis and battery research. The first focus is new materials architectures for catalytic materials for bond-specific activation for efficient chemical transformations. Practical implications range from more energy efficient and environmentally friendly strategies for chemical synthesis to the replacement of current petrochemical feedstocks by inexpensive abundant small alkanes. The second area is electrical energy storage where the development of revolutionary new materials for energy storage is a key to solving the nation's energy problems. Here the project will focus on new materials for the interface between electrolyte and electrode, i.e., the solid-electrolyte interface (SEI), which involves many of the same materials design principles as catalytic materials, including activity and stability. This will have practical applications such as safer lithium ion batteries for electric vehicles and new battery technologies for long range electric vehicles.

2010 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: "Prototype Ultra High-Resoluation Climate-Weather Modeling Studies"

Principal Investigator: S.-J. Lin, NOAA Geophysical Fluid Dynamics Laboratory
Co-Investigators: Christopher Kerr, NOAA Geophysical Fluid Dynamics Laboratory

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 25,000,000 processor hours

Research Summary:
This project will explore the frontier of weather predictions and climate modeling with the newly developed Geophysical Fluid Dynamics (GFDL) global cloud-resolving model with bulk micro-physics at approximately 12 km resolution (hydrostatic configuration) and 4.5 km resolution (non-hydrostatic configuration). Over the last year, considerable progress has been made on improvements to the Flexible Modeling System (FMS) infrastructure for GFDL, especially with regard to I/O scaling. The model will be validated for stability and dynamical formulation and then with full-physics. Hurricane hindcast experiments will be used to test short-term prediction (especially of hurricane track and intensity). Regional fidelity of the 12 km GFDL will be tested with multiple Atmospheric Model Intercomparison Project (AMIP) -type runs. These long term runs will be used to compare simulation to actual data for 2008.

Title: "Simulation of Large Conformational Transitions in Macromolecular Systems using Leadership Computing"

Principal Investigator: Benoit Roux, University of Chicago/ Argonne National Laboratory

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 28,500,000 processor hours

Research Summary:
Atomistic molecular dynamics (MD) simulations are increasingly helping to understand complex macromolecular systems; however, many questions cannot be addressed with simple "brute force" MD simulation methods. For example, study of large-scale motions in macromolecules requires special methods and strategies on leadership computing resources. This project will develop novel and cutting-edge approaches based on the string method with swarms-of-trajectories and Milestoning with a complete Voronoi tessellation for characterizing complex conformational transitions in large macromolecular systems. The project goal is that the core of the study will serve as a future road-map for simulating, visualizing and elucidating the reaction mechanics of large macromolecular nano-machines. These techniques are general and could be applied to determine the pathway controlling interaction of cellulose with its substrate, an important step to engineer better ethanol production strategies. In this project the methods will be used to compute the transition pathway for activation of the voltage-gated Kv1.2 channel. Voltage-gated Potassium (Kv) channels can switch between different conformational and functional states, a process known as "gating", thereby allowing or blocking the passage of ions across the cell membrane in response to various cellular signals. Kv channels are among the most well-characterized molecular machines using a wide range of experimental methods (yet many outstanding issue remain). A voltage-gated membrane channel is a functional device that could be integrated in the design of artificial switches in various nanotechnologies.

Title: "Direct Multiobjective Optimizaton of Storage Ring Lattices for the APS Upgrade and Beyond"

Principal Investigator: Michael Borland, Argonne National Laboratory

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 36,000,000 processor hours

Research Summary:
The Advanced Photon Source (APS) is a third-generation, 7-GeV storage ring light source that has been in operation for well over a decade. It is currently one of the brightest sources of x-rays in the world. An upgrade is under consideration that would involve significant changes to the configuration of the magnets (the "lattice") in order to provide additional features for x-ray users. Proposed changes would allow longer insertion devices (increasing x-ray brightness by an order of magnitude for energies above 20 keV), and reducing x-ray pulse length by several orders of magnitude (securing a unique position for APS in enabling time-resolved science with hard x-rays). However, all these changes must be made without adversely impacting existing operating modes, beam intensity, and other performance measures. This project will use nonlinear dynamics simulations to address design issues such as sufficient dynamic aperture (to ensure high injection efficiency) and momentum aperture (to ensure sufficient beam lifetime).

Title: "Nucleon Structure down to the Physical Pion Mass"

Principal Investigator: John Negele, Massachusetts Institute of Technology

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 37,800,000 processor hours

Research Summary:
This project will exploit a unique opportunity to perform the first calculation of nucleon structure using full lattice QCD at the physical pion mass. The recent calculation of the hadron spectrum by the Budapest-Marseille-Wuppertal (BMW) collaboration broke new ground in developing the action and computational technology highly optimized for the BG/P. Given the highly recognized success of this action, it is extremely attractive to utilize this same approach to calculate nucleon form factors, moments of structure functions, and generalized form factors down to the physical pion mass. It is expected that these pioneering structure calculations down to the physical pion mass will achieve key strategic goals of the U.S. lattice QCD effort, and will have significant impact on the national DOE nuclear physics experimental program.

Title: "Scalable, Explicit Geometry, Whole Core Nucelar Reactor Simulations"

Principal Investigator: Micheal Smith, Argonne National Laboratory
Co-Investigators: Allan Wollaber, Los Alamos National Laboratory
Dinesh Kaushik, Argonne National Laboratory
Won Sik Yang, Argonne National Laboratory
Elmer Lewis, Northwestern University

ALCC allocation:
Site: Argonne National Laboratory
Allocation: 38,000,000 processor hours

Research Summary:
As part of the U.S. DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, a multi-physics simulation framework named SHARP (Simulation-based High-efficiency Advanced Reactor Prototyping is being developed specifically for the analysis and design of sodium cooled fast reactors. Accurate prediction of the reactivity feedback due to core radial expansion, which is very important for the design and safe operation of a reactor, is one of the most challenging multi-physics simulation problems, requiring coupled neutronics, thermo-fluids and structural analyses. This simulation requires the UNIC neutronics code to produce accurate power distributions for deformed geometries. Although UNIC has shown its capability to produce very detailed solutions, these must be validated against experiments before UNIC is fully coupled with thermo-fluid and structural analysis codes. This project will analyze the detailed reaction rate distributions measured in a full-scale critical experiment carried out in the ZPR-6 facility for the validation. Initial runs of a ZPR-6 Assembly 6A model using 1.7 million serendipity quadratic hexahedral elements, 160 angular directions, and 9 energy groups (approximately 50 billion degrees of freedom) were performed on BlueGene/P using up to the whole machine. To obtain accurate, locally detailed solutions, indications are that more than 100 energy groups will be necessary, along with at least 1.4 times as many vertices –an order of magnitude increase in the problem size. Ongoing preconditioner development in UNIC to reduce the memory burden and improve per processor performance will allow us to execute these calculations using the BlueGene/P machine at Argonne National Laboratory.

Title: "A Center for Turbulence Research -- Argonne Leadership Computing Facility Collaboratory for Very Large Scale Turbulence Simulatoins on Petascale Computing Platforms"

Principal Investigator: Parviz Moin, Stanford University
Co-Investigators: Ramesh Balakrishnan, Argonne National Laboratory,
Rick Stevens, Argonne National Laboratory,
Paul Messina, Argonne National Laboratory,
Pete Beckman, Argonne National Laboratory,
Katherine Riley, Argonne National Laboratory,
Raymond Bair, Argonne National Laboratory

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

Research Summary:
Since its founding in the 1980s, the Center for Turbulence Research (CTR) has stimulated significant advances in the physical understanding of turbulence and related non-linear multiscale phenomena through the development and application of advanced numerical simulation techniques on massively parallel platforms. As an international focal point of key turbulence research, CTR leads the development of new concepts for turbulence control and modeling of complex effects on turbulence including the effects of complex geometry, multi-material mixing, chemical reactions, complex fluids, multiphase flow, shock waves, magnetohydrodynamics, heat transfer, acoustics and aero-optics.

These key advances in turbulence simulation were made possible through sustained interactions between researchers and computational scientists employing high-powered computing resources. The proposed collaboration between CTR and the Argonne National Laboratory represents such a unique combination of numerical analysts, engineers, and computational scientists able to accelerate major scientific discoveries and engineering breakthroughs in turbulence physics by expanding the known boundaries of what is possible on emerging parallel architectures and significantly broadening the community of researchers capable of using leadership-class computing resources.

Title: "Improving Light Water Reactor Fuel Reliability Via Flow Induced Vibration Simulations"

Principal Investigator: Andrew Siegel, Argonne National Laboratory
Co-Investigators: David Pointer, Argonne National Laboratory
Paul Fischer, Argonne National Laborator

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

Research Summary:
Failures of the fuel rod elements which power U.S. nuclear plants are rare. One of the common causes of these rare failures is flow induced vibration of fuel assembly components. Indeed, the Electric Power Research Institute reports that more than 70% of all fuel failures in the U.S. pressured water reactor fleet occur as a consequence of grid-to-rod fretting. This project will investigate vibrations caused by turbulent flow in the core of light-water reactors. The inability to accurately predict and understand vibrations and contact-induced mechanical wear of spacers on fuel rods in light-water reactor (LWR) cores has been identified by utilities and fuel vendors as a major cause of fuel failure and a bottleneck to optimal fuel utilization. This work will be done in conjunction with a larger Nuclear Energy Hub effort that aims to develop a toolbox of simulation and modeling tools for nuclear reactor design and operation.

Title: "Stochastic Nonlinear Data-Reduction Methods with Detection & Prediction of Critical Rare Events"

Principal Investigator: Guang Lin, Pacific Nortwest National Laboratory
Co-Investigators: Eric Vanden-Eijnden, Courant Institute
George Em Karniadakis, Brown Universitym
Xiaoliang Wan, Louisiana State University

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

Research Summary:
Data-driven simulations at the petascale level could lead to great advances in predicting accurately the performance of dynamic data-driven application systems (DDDAS), but the main bottleneck is the ability to deal effectively with the petascale outputs of these unsteady simulations. In addition, the uncertainty associated with the simulation inputs may render the results of these highly expensive simulations erroneous, especially in long-term predictions. This project will address three specific current limitations in modeling stochastic systems: (1) The inputs are mostly based on ad hoc models, (2) The number of independent parameters is very high, and (3) Rare and critical events are difficult to capture with existing algorithms. To overcome these problems the project will research three topics: (1) Development of certified low-dimensional models for effective reduction of dimensionality, (2) Development of a scalable sensitivity-based hierarchical uncertainty quantification (UQ) approach, and (3) Development of algorithms for real-time anomaly detection and rare events prediction. Although the focus here is on atmospheric sciences, this comprehensive new mathematical and computational framework for data analysis of petaflop stochastic simulations can be used across many disciplines. Applying the framework on large-scale climate data sets and global climate models will help advance understanding of the low-dimensional behavior and transient response of the Earth system to different climate forcings and better predict future climate changes.

2010 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: "ASCR Joule Metric"

Principal Investigator: Kenny Roche, Pacific Northwest National Laboratory
Co-Investigators: Doug Kothe, Oak Ridge National Laboratory
Aurel Bulgac, University of Washington
Lin -Wang Wang, Lawrence Berkeley National Laboratory
Thomas Evans, Oak Ridge National Laboratory
Phil Jones, Los Alamos National Laboratory
Mat Maltrud, Los Alamos National

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

Research Summary:
The Office of Advanced Scientific Computing Research's (ASCR) Joule Software Metric for Computational Effectiveness is to "improve computational science capabilities, defined as the average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes. FY10 performance metric: efficiency measure is ≥100%." Ensuring compliance with these metrics, which are tracked on a quarterly basis, is an important milestone each fiscal year for the DOE ASCR Program Office as well as for the success of the overall DOE SC-1 open science computing effort. For FY10, the four Joule application codes are TD_SLDA, software used to describe the response of superfluid systems to any external time-dependent probe within an extension of the density functional theory (DFT); LS3DF, a divide-and-conquer code for density functional theory (DFT) level ab initio self-consistent calculations of nano-systems; DENOVO, a three-dimensional, linear radiation transport code that is designed to support shielding analysis, medical physics, nuclear criticality, homeland defense and nuclear safeguards, and nuclear reactor design; and POP, ocean circulation model that solves the three-dimensional primitive equations for fluid motions on the sphere under hydrostatic and Boussinesq approximations. ALCC time is used to collect benchmark data the codes , to enhance the efficiency, scalability and science capability of the application software and a limited set of science runs

Title: CASL: The Consortium for Advanced Simulation of Light Water Reactors – A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

Principal Investigator: Doug Kothe, Oak Ridge National Laboratory
Co-Investigators: Ronaldo Szilard and Richard Martineau, Idaho National Laboratory,
Paul Turinsky and Dan Cacuci, North Carolina State University,
Mario Carelli and Zeses Karoutas, Westinghouse Electric Company,
John Gaertner, Electric Power Research Institute,
John Turner and Jess Gehin ,Oak Ridge National Laboratory,
Chris Stanek and Ed Dendy ,Los Alamos National Laboratory,
Mujid Kazimi and Sid Yip, Massachusetts Institute of Technology, Bill Martin, University of Michigan,
Jim Stewart and Randy Summers, Sandia National Laboratories, Dan Stout, Tennessee Valley Authority

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

Research Summary:
The Consortium for Advanced Simulation of Light Water Reactors (CASL) will apply existing modeling and simulation (M&S) capabilities and develop advanced capabilities to create a usable environment for predictive simulation of light water reactors (LWRs). This environment, designated the Virtual Reactor (VR), will:

- Enable the use of leadership-class computing for engineering design and analysis to achieve reactor power uprates, life extensions, and higher fuel burnup.
- Promote an enhanced scientific basis and understanding by replacing empirically based design and analysis tools with predictive capabilities.
- Develop a highly integrated multiphysics M&S environment for engineering analysis through increased fidelity methods [e.g., neutron transport and computational fluid dynamics (CFD) rather than diffusion theory and subchannel methods].
- Incorporate UQ as a basis for developing priorities and supporting application of the VR tools for predictive simulation.

CASL will focus on a set of challenge problems that encompass the key phenomena limiting the performance of PWRs, with the expectation that much of the capability developed will be applicable to other types of reactors. Broadly, CASL's mission is to develop and apply M&S capabilities to address three critical areas of performance for nuclear power plants (NPPs):

- capital and operating costs per unit energy, which can be reduced by enabling power

uprates and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new Generation III+ NPPs;
- nuclear waste volume generated, which can be reduced by enabling higher fuel burnups; and
- nuclear safety, which can be enhanced by enabling high-fidelity predictive capability for component performance through failure.

Work to develop the VR will be executed in five focus areas (FAs) selected to ensure that the VR: (1) is equipped with the necessary physical and analytical models and multiphysics integrators; (2) functions as a comprehensive, usable, and extensible system for addressing essential issues for NPP design and operation and; (3) incorporates the validation and UQ needed for credible predictive M&S.

To deliver on its mission, CASL will place near-term priority on improved simulation of the reactor core, internals, and vessel for a pressurized water reactor (PWR). The developed capability will be tightly coupled to an existing and evolving out-of-vessel simulation capability. Much of the CASL VR to be developed will be applicable to other NPP types, in particular boiling water reactors (BWRs). During its later years of operation, CASL activities will expand to include structures, systems, and components (SSC) beyond the reactor vessel and will more directly consider BWRs and small modular reactors (SMR).

Title: "AR-5 Calculations"

Principal Investigator: Jim Hack, Oak Ridge National Laboratory
Co-Investigators: Peter Gent, National Center for Atmospheric Research
V. Balaji, National Oceanic and Atmospheric Administration /Geophisical Fluid Dynamics Laboratory

ALCC allocation:
Site: Oak Ridge National Laboratory
Allocation: 80,000,000 processor hours

Research Summary:
The IPCC Assessment is the most visible international science activity dealing with global climate change; it informs climate-change policy and the direction of research within the participating nations. It is clearly very important for the US to make a leading contribution in terms of the simulation quality and complexity. The fifth assessment report (AR5) of the Intergovernmental Panel on Climate Change (IPCC) is scheduled to be published in early 2013. This report can only assess papers that are either published in peer reviewed journals, or accepted for publication. Therefore, the complete suite of AR5 runs must be finished by the end of December, 2010. ALCC hours will be used to support the NSF/DOE Community Climate System Model (located and managed at NCAR) and GFDL's AR5 efforts.

The NCAR CCSM project will use ALCC time to conduct a series of high resolution ($1/4^o$) CMIP5 time slice experiments with the newly released CAM4. These simulations will be coordinated with similar DOE and NOAA efforts. The goal will be to simulate the past 20 years using observed SSTs (AMIP), along with multidecadal simulations that include the SST/sea ice changes (anomaly experiments) from a lower resolution CCSM4 climate change experiment. This team will also conduct a pre-industrial control, 20th century ensemble, and future representative concentration pathways (RCP) ensemble experiments (to year 2100) with newly released Community Earth System Model (CESM) at 1^o horizontal resolution in the atmosphere. This will allow a model, which includes much more sophisticated physics treatments and five times the operation count, to be assessed in the context of its predecessor at a resolution that provides for a superior treatment of the large-scale dynamical circulation.

The GFDL proposes to use ALCC resources to perform model simulations also targeted at the CMIP5 experimental suite (the framework for the AR5). GFDL anticipates using this resource in CY10 to perform experiments along two streams: time-slice experiments that focus on regional US climate change and coupled model experiments that expose the role of the ocean in climate variability and change. These scientific goals align directly with those of the IPCC's 5th Assessment Report (AR5). Reaching them will depend on scientific validation of existing models within the DOE environment, as well as priority access to the computing resources. When successful, the data from these experiments will be made available in a form consistent with AR5 protocols and other user-friendly forms for consumption by the climate impacts community.

Title: "Exascale Computing for Accelerating Deployment of Retrofittable CO2 Capture Technologies via Simulation Tools with Quantified Uncertainty"

Principal Investigator: Philip Smith, Univeristy of Utah /Institute for Clean and Secure Energy (ICSE)

ALCC allocation:
Site: Lawrence Berkeley National Laboratory
Allocation: 3,200,000 processor hours

Research Summary:

There is an increasing awareness in the U.S. that an effective, sustainable response to climate change must include cost-effective retrofit technologies to reduce carbon dioxide emissions from large stationary sources such as coal-fired power plants. We need economically viable retrofit technologies that will improve carbon dioxide capture efficiency, utilize or store the carbon dioxide produced, and simultaneously reduce criteria pollutants and water contaminants. Full-scale predictions with known uncertainties and errors, produced by simulation science coupled with modern measurement and monitoring methods, have the potential to provide more rapid deployment of carbon dioxide retrofit technologies. This project will employ a validation/uncertainty quantification methodology that provides upper and lower bounds on a predicted quantity of interest by requiring consistency between simulation output and experimental data. This methodology will be applied in two specific areas of carbon dioxide retrofit technologies: oxy-fuel firing and carbon dioxide mineralization.

Title: "Large scale particle-in-cell simulations of laswer-plasma interactions relevant to Inertial Fusion Energy (IFE)"

Principal Investigator: F. S. Tsung, University of California, Los Angeles
Co-Investigators: W. B. Mori, University of California, Los Angeles

ALCC allocation:
Site: Lawrence Berkeley National Laboratory
Allocation: 3,250,000 processor hours

Research Summary:
This project will use the UCLA collection of particle-in-cell (PIC) simulation codes to study laser and particle transport through plasmas. Laser plasma interaction is important to inertial confinement fusion, stockpile stewardship, inertial fusion energy (IFE), and is a fundamental topic within the field of high-energy density science. Recently, the National Ignition Facility (NIF) delivered one mega-joule on target for the first time ever, while other higher gain IFE schemes like shock ignition are being pursued in laser facilities such as OMEGA. This project will study high frequency laser-plasma instabilities that can absorb, deflect, or reflect laser light, and generate energetic electrons. Such processes can limit the laser intensity in both direct and indirect drive IFE scenarios, thereby limiting the overall gain. In conventional IFE the fast electrons can preheat the target, hinder compression, and hence reduce yield. Two important instabilities are two-plasmon decay and stimulated Raman Scattering (SRS). The project will tackle 2D simulations of: SRS involving multiple speckles or multiple laser beams at an oblique angle, two Plasmon decays with overlapping laser beams, and fast electron generations and transport in shock ignition scenarios.

Title: "First Principles Design of Advanced Thermal Energy Storage Materials"

Principal Investigator: Su-Huai Wei, National Renewable Energy Laboratory
Co-Investigators: Joongoo Kang, National Renewable Energy Laboratory, Junyi Zhu, National Renewable Energy Laboratory

ALCC allocation: 5,000,000 Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 5,000,000 processor hours

Research Summary:
Solar thermal electricity generation has great potential as a renewable energy source. To achieve the full potential of this system requires revolutionary advances in the energy storage capacity and stability of heat storage media. Nanoscale "capsule" structures containing solid/liquid or solid/gas phase change materials (nanoPCMs) have been proposed as novel thermal energy storage media. NanoPCMs offer several advantages over conventional bulk storage systems: enhanced heat transfer rate due to high surface-to-volume ratio, tunability of phase-transition temperatures that depend on the system size. However, for the design of efficient thermal storage materials, we first need to understand how the melting transition occurs in such encapsulated nanoscale systems. This project will perform large-scale, first-principles molecular dynamics (MD) simulations to advance fundamental understanding and unravel the microscopic phase change mechanisms of nanostructured materials. Simulations will focus on characterizing the melting behaviors of (1) metal nanoalloy and salt nanoparticles, (2) metal/oxide core-shell structures, and (3) nanoparticles confined in porous solid materials. Heat capacity of nano-composite systems will be calculated to address key thermodynamic quantities such as melting point and heat of fusion. The project will also establish the effect of core-shell interactions on the phase transition and thermal stability, providing conceptual breakthroughs in thermal storage for concentrating solar thermal systems.

Title: "A multi-decadal reforecast data set to improve weather forecasts for renewable+ energy applications"

Principal Investigator: Thomas Hamill, NOAA Earth Research Laboratory
Co-Investigators: Jeffrey Whitaker, NOAA Earth System Research Laboratory

ALCC allocation:
Site: Lawrence Berkeley National Laboratory
Allocation: 14,500,000 processor hours

Research Summary:
This project will generate a next-generation multi-decadal "reforecast" data set. The reforecast data set will spur the development of novel longer-lead weather forecast applications for renewable energy, such as several-days lead and even week-2 forecasts of the potential for wind-energy generation and incoming solar radiation, as well as heavy precipitation and streamflow into reservoirs generating electrical power. A reforecast is a retrospective forecast of the weather, performed using a weather forecast model that is used operationally. Since numerical weather predictions are affected both by the chaotic growth of errors during the forecast and by model deficiencies, the use of direct model output for making weather-related decisions can lead to poor decisions. However, it has been demonstrated that it is possible to statistically extract the useful meteorological signal from the chaotic noise and model error in the direct model output and produce skillful and reliable forecasts useful to a wide range of customers. This new reforecast data set, using a forecast model operational in 2010 will allow NOAA to develop a whole range of new and more accurate weather forecast applications for renewable energy.