2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Designing Bioinspired Catalysts for Energy Harvesting & Renewable Energy.

Principal Investigator: Pratul Agarwal, Oak Ridge National Laboratory (ORNL)

Co- Investigator: Chakra Chennubhotla, University of Pittsburgh

Allocation: 5 million processors hours

Research Summary:

Bio-inspired rational catalyst design through joint computational-experimental effort has important implications for DOE's mission in renewable energy. Catalysts have been sought for degradation of cellulose in biomass to fermentable sugars for production of low-cost bio-ethanol as a renewable energy source. Further biochemical processes that allow solar energy harvesting have also been sought for improved carbon assimilation strategies. Biological catalysis mediated by enzymes offers advantages including high substrate specificity, high catalytic efficiency and low-cost. Bio-inspired or bio-mediated catalysts at industrial level has had limited impact, particularly in the area of renewable energy. Significant challenges are almost always encountered in achieving the goals of retaining enzyme activity after modifications, and designing more efficient enzymes, as the knowledge of underlying engineering design parameters still remains missing. We hypothesize that theoretical/ computational modeling driven experimental strategies could play a vital role in investigating bio-catalytic processes mediated by enzymes, and have the potential to lead to the development of highly efficient bio-mediated catalysts. We are currently using the following steps for developing new bio-catalysts for renewable energy:

Aim 1: Understanding kinetics and efficiency of enzyme mediated bio-catalytic processes. Theoretical and computational models are being developed for understanding the factors that control the efficiency of enzyme mediated bio-catalytic processes. Based on the output from these computational models, mutations and modifications are being proposed for the enzyme engineering strategies to develop
highly efficient bio-catalysts.

Aim 2: Engineering highly efficient bio-catalysts for renewable energy. Cellulases have attracted interest for use in low-cost production of bio-ethanol as a renewable source of energy. We have already developed a computational model for the catalytic activity of cellulase Cel9A from *Thermobifida fusca.* New bio-catalysts based on engineered Cel9A are being experimentally developed and validated.

Aim 3: Novel methodology for bio-mediated light energy harvesting. We are also exploring methodology for developing hyper-catalytic enzymes for improving metabolic flux at critical bottle-necks points in the cellular metabolism, with the long term goal of increasing the biomass yield as well as large scale industrial applications for light (solar) energy harvesting.

Our computational methodology is based on the use of molecular dynamics (MD). Building upon the preliminary success, we continue to pursue theoretical & computational modeling driven investigations of bio-catalytic processes. Specifically we are focusing on: developing computational methodology for identification of conformational sub-states; identification of structural and conformational factors that affect the catalytic efficiency and applying the developed methodology to investigate cellulase Cel9A from *Thermobifida fusca* and RuBisCO from *Rhodospirillum rubrum.*

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Petascale Atomistic Simulations of Ultra Scaled Transistors.

Principal Investigator: Behtash Behin-Aein, Global Foundries

Co- Investigator: Bhagawan Sahu, Global Foundries

Allocation: 8 million processors hours

Research Summary:

In the last few decades, transistor scaling and subsequent increase of the density of electronic devices per unit-area have made computers more powerful and also cheaper while retaining upper limits on the energy dissipation. This has been made possible mainly because each transistor has become more energy efficient. However, enhancing the device performance and reducing the energy consumed (in both ON and OFF states of a transistor) is becoming a daunting challenge. The power dissipation per transistor is believed to be the single most important impediment to continued miniaturization and there is a serious attempt to "*reinvent the transistor*" so as to operate them at lower voltages. The focus of this project is to investigate ultra scaled transistors with novel channel materials i.e. SiGe alloy with various random Ge concentrations and strain in order to improve the performance thereby reducing the energy consumption. We will model the 3-dimensional quantum hole or positive charge transport in FinFET device geometry with SiGe alloy. We anticipate 25% energy savings per transistor by improving hole mobility in SiGe only. Based on published data for 2010 when data centers used up between 1.7-2.2% of all electricity in the USA, we can estimate that our targeted 25% energy saving from novel channel material for semiconductors will result in more than 0.8% reduction in total electricity used in the country for data centers alone. As the device sizes shrink more, we are ushering into a new era where the transport characteristics and hence the device performance depend on many properties at the atomic scale. The atomistic nature of the channel as well as the interfaces or junctions will then play a critical role in performance improvements. Traditionally used semi-classical transport models for semiconductor devices are not sufficient to capture all the physics of ultra scaled transistors and introduction of new channel materials other than Si such as SiGe poses a complex task especially when no hardware/experimental test structures is available in semiconductor industries. Modeling of nano-scale devices require a quantum mechanical description that takes into account electronic structure of new materials and alloy along with an *appropriate* quantum transport formalism. Such quantum mechanical descriptions of nano-scale devices impose significant modeling and computing challenges while promising predictive capabilities for new device architectures with novel materials. For realistic device sizes, atomistic simulations of electronic structure coupled with electrical transport, at the device level is now possible with materials containing more than one element such as SiGe with Ge occupying Si positions in a random fashion. (SiGe alloy is emerging as a novel channel material for the positive charge carrier transport in future complementary metal oxide semiconductors namely CMOS.) The development of more energy efficient semiconductor devices, in turn , will increase the energy efficiency of consumer electronics such as computers; cell phones and electronics in the automotive industry that use semiconductors circuits and sensors and other niche applications, thereby helping DOE advance a clean energy agenda for the nation. The research also explores new frontiers in understanding quantum mechanical effects such as tunneling, state quantization, and atomistic disorder at the nano scale which can lead to emerging new phenomena not observed before. While the total number of desktops and laptops in the USA are not known, we can estimate their number by sales figures that are approaching 100,000,000 units a year that includes the fast growing tablet market. We guess that computer upgrading cycle is closer to three years now, which gives us an estimate of 300,000,000 stand-alone computers. The energy savings our technology will provide will result in 100kWh saving per computer, which exceeds 1% electricity savings per capita. We think that our conservative estimates based only on high performance applications in computational devices will bring close to 2% saving in national electricity consumption.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Time Dependent Density Functional Theory (TDDFT) Approach to Nuclear Reactions.

Principal Investigator: Aurel Bulgac, University of Washington

Co- Investigators: Kenneth Roche, University of Washington; Ionel Stetcu, Los Alamos National Laboratory (LANL); C. Bertulani, Texas A&M; and P. Magierski, University of Washington

Allocation: 12 million processors hours

Research Summary:

We have combined the latest developments in DFT (Density Functional Theory), the (TD)SLDA ((Time-Dependent) Superfluid Local Density Approximation), with the best computer science methods for leadership class computers. We will use our software to describe nuclear structure, nuclear reactions and ultimately induced fission in a unified formalism within appropriate validated extensions of the DFT applied to nuclear systems. This major theoretical advance will lead, for the first time, to a microscopically consistent description of nuclear reactions in medium and heavy nuclei. Our software solves tens to several hundreds of thousands of coupled nonlinear TD 3D partial differential equations. We will study the real-time 3D dynamics without any restrictions in very large nuclear volumes of the order of 80^3 fm^3 and time intervals up to 10^{-20} …10^{-19} sec.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Generation of Intrinsic Toroidal Rotation in Tokamak Plasma to enable Stable Fusion Energy Production.

Principal Investigator: Choong-Seock Chang, Princeton Plasma Physics Laboratory (PPPL)

Co- Investigators: S. Ku (PPPL), D. Stotler (PPPL), Scott Klasky (ORNL), and Scott Parker, University of Colorado

Allocation: 20 million processors hours

Research Summary:

We will perform comprehensive first-principles gyrokinetic simulations to understand how tokamak plasma can generate a spontaneous toroidal rotation without an explicit external momentum input, such as neutral beam injection, as observed in the experiments for over a decade but with only an illusive understanding of the underlying physics mechanism. Thermonuclear fusion reactors can be discussed only after the plasma is brought to stable equilibrium state. It has been found experimentally and theoretically that a moderate level of toroidal plasma rotation could bring the plasma into a stable equilibrium state. In ITER and fusion reactors which contain much more massive and higher pressure plasma than today's small tokamaks do, an external momentum input by neutral beam becomes negligibly small since the beam momentum increases only as square-root of beam energy, while the maximal neutral beam energy is limited by the volume ionization requirement. Hence, plasma rotation generation in ITER plasma needs to rely upon a spontaneous mechanism. However, an axisymmetric toroidal plasma conserves total toroidal momentum. A spontaneous rotation generation requires a physical mechanism to exchange momentum with the external world. Without a validated physics understanding, extrapolation of the present experimental data to ITER contains too much uncertainty. This study will focus on the momentum source in the tokamak edge, by considering the edge plasma interaction with the external world through the magnetic separatrix coil and the material wall. The comprehensive gyrokinetic code XGC1 will be used in a realistic tokamak geometry containing material wall, magnetic separatrix, and wall-recycled neutral particles from first principles. Redistribution of the edge momentum into the plasma core will also be studied. A multi-peta flop HPC Jaguar/Titan will be utilized. This study will not only make it possible to obtain an in-depth understanding of the spontaneous rotation generation, but also to provide physics-based improvement to the purely empirical scaling formula for spontaneous rotation and to increase its confidence in predicting the stable operation window of ITER and future fusion reactors.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Projections of Ice Sheet Evolution Using Advanced Ice and Ocean Models.

Principal Investigator: William Collins, Lawrence Berkeley National Laboratory (LBNL)

Co- Investigators: Daniel F. Martin (LBNL), Esmond G. Ng (LBNL), Michael F. Wehner (LBNL), Woo-Sun Yang (LBNL), Xylar S. Asay-Davis (LANL), Philip W. Jones (LANL) , William H. Lipscomb (LANL), Matthew Maltrud (LANL), Stephen F. Price (LANL), Stephen L. Cornford (University of Bristol), and Anthony J. Payne (University of Bristol)

Allocation: 13 million processors hours

Research Summary:

Mass loss from the Greenland and Antarctic ice sheets is accelerating. As the Earth's climate warms, there is a risk of abrupt retreat of marine-based ice sheets, resulting in rapid sea-level rise. Until recently, ice sheet models were relatively crude and were not included in climate models. As a result, projections of 21st century sea-level rise are highly uncertain and may be too low. There is an urgent need to advance our understanding of the mass balance, dynamics, and thermodynamics of ice sheets and their interactions with other parts of the climate system, especially the ocean. Recent scientific and computational advances have made it possible to simulate ice sheet evolution on high-performance computers with unprecedented grid resolution and physical realism.. Scientists at Lawrence Berkeley National Laboratory (LBNL), working in collaboration with researchers at Los Alamos National Laboratory (LANL) and the University of Bristol, have developed novel methods for simulating ocean circulation and heat exchange beneath advancing and retreating ice shelves. As a result, we are now able to model whole ice sheets with sophisticated dynamics on annual to millennial time scales and with ultra-high resolution focused on fast-moving regions, where dynamical length scales are 1 kilometer or less. The award involves first-of-a-kind simulations which will provide improved estimates of the rate of retreat of marine ice sheets during the next several decades

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Protein Folding and Computational Models.

Principal Investigator: Ken Dill, Stony Brook University

Co- Investigators: Michael McGuigan, Brookhaven National Laboratory (BNL), Evangelos Coutsias (University of New Mexico), Alberto Perez (Stony Brook University), Yan Li (BNL), and Justin MacCallum (Stony Brook University)

Allocation: 2 million processors hours

Research Summary:

This project aims at reducing the cost for obtaining 3D protein structures, which are vital for deriving new drug-like compounds to combat disease. In the recent years, a vast amount of protein sequence information has come from genome sequencing projects, but the sequence alone is not enough to find cures for disease. Protein structures are needed, but they are costly to obtain. A recent publication explains that the experimental cost of obtaining protein crystals from which to derive protein structure surpasses even the price of diamonds. The process is also time consuming, so the gap between known sequences and structures grows larger every year. We are going to use massively efficient parallel GPU molecular dynamics simulations methods in combination with sparse bioinformatics information in order to derive the structure of proteins. Based on previous results we expect to cut down the time to obtain structures from the year time scale to the month scale. The process will also be much cheaper. Additionally, we plan to use quantum mechanics derived potentials to improve the efficiency and accuracy of protein molecular dynamics.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Impact of the Inlet Boundary Condition on High-Pressure Turbine Temperature Predictions

Principal Investigator: Anne Dord, General Electric

Co- Investigators: N/A

Allocation: 34 million processors hours

Research Summary:

The components of the aircraft engine cycle (i.e. compressor, combustor, and turbine) operate close to their efficiency limits. Reducing fuel consumption, increasing the life of an engine, and reducing cost are all challenges for modern engine manufacturers. Compressor, combustor, and turbine subsystems must be designed to meet stringent efficiency, durability and emission requirements. It is well understood that optimizing the engine must be done at the system level. For example, increasing the combustion temperature will increase the thermal efficiency but will also cause higher thermal stresses and thus shorten the life of the high pressure turbine. These tradeoffs are very important and must be considered during the design process. However, components are often studied in relative isolation from one another and important interaction effects can be lost. At the combustor and turbine interface, complex flows and extreme conditions exist consisting of high temperature gas, variable boundary layers, unsteady leakage and cooling flows, and turbulence. The culmination of these physics plays an important role in both the combustor and turbine performance. Over the past decade, progress has been made in numerical modeling of multiphysics flows for gas turbine and aircraft engine applications. Large Eddy Simulations for complex combustor simulations are now commonly found in the literature. These simulations are often limited to the combustor itself and few take into account the stage one vane. Recent studies show that not adding the stage one vane impacts the exit temperature profile (used to guide turbine design) and thus turbine durability and performance predictions. Among the different strategies proposed to couple the combustor and high pressure turbine, very few are of high fidelity and often ignore important aspects like cooling. In this study, an alternate strategy is proposed to investigate the combustor-turbine interface. Based on the assumption that the feedback effect from the turbine is concentrated to the vicinity of the combustor exit, only the downstream part of the combustor is considered. The mesh is built so as to enable an accurate description of the large scale eddies traveling towards the combustor exit and into the high pressure vane. Large eddy simulations (LES) of the coupled domain, using explicit solvers would address the following outstanding questions for turbine designers:

- What is the influence of the stage one vane on the exit temperature profile?
- What is the influence of the stage one vane on the incoming velocity profile?
- What is the impact of using a mean temperature profile for turbine design as opposed to a transient?
- What is the benefit of using LES in the stage one vane ?

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Liquid-solid interfaces in electrocatalysis from first principles.

Principal Investigator: Jeffrey Greeley, Argonne National Laboratory (ANL)

Co- Investigators: Subramanian Sankaranarayanan, ANL

Allocation: 20 million processors hours

Research Summary:

The research will leverage new, highly parallelizable electronic structure Density Functional Theory (DFT) codes to determine critical aspects of the electrocatalytic properties of transition metal/water interfaces for selective deNOx reactions. The properties of liquid/solid interfaces, in general, are only beginning to be explored with first principles methods, and the electrochemical processing of nitrogen-containing pollutants, in particular, is a novel strategy for environmental catalysis that is poorly understood at the atomistic level. This study will be one of the first uses of electronic structure methods that combines rigorous modeling of solid/liquid interfaces with detailed mechanistic analysis of electrochemical deNOx chemistry to both understand and, ultimately, propose new catalysts for this novel electrocatalytic process. The approach focuses on a combination of reaction network analysis and ab initio molecular dynamics (AIMD) simulations, many of which will require very long time scale runs to obtained converged properties, to elucidate the key physical and catalytic properties of the electrochemical deNOx chemistry.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Controlling Nanoparticle Assembly to Engineer New Materials.

Principal Investigator: Gary Grest, Sandia National Laboratories (SNL)

Co- Investigators: Sanat Kumar (Columbia), Dvora Perahia (Clemson), Steve Plimpton (SNL), Mark Robbins (Johns Hopkins), and Mark Stevens (SNL)

Allocation: 30 million processors hours

Research Summary:

The pathways to control assembly and integration of nanoparticles (NPs) into new devices will be probed using multi-million atom molecular dynamics simulations. The potential of NPs has been long realized however imbedding them in different devices remains a challenge. Our study will address the major barriers to integrating NPs into a range of advances devices, controllably dispersing and organizing them within durable matrices while retaining their unique properties. The research will utilize the building blocks and methodology derived in the previous allocation to understand the forces that control the symmetry of assemblies and correlate them with the properties of the systems. NPs encoded with organic ligands that allow control of the strength, length scale and directionality of the inter-particle interactions will be investigated. The current study will zoom into the interaction regions, providing the needed molecular level understanding of the assembly process. Combining fully atomistic and coarse grained simulations we will correlate the interactions between NPs and between NPs and their surroundings with the properties of NP assemblies.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Supercomputer Enabled Accelerated Development of Revolutionary Supersonic Shock Wave Based Turbomachines: Achieving DOE Goals for Compressing Carbon Dioxide and Achieving High Energy Efficiency via High Resolution CFD.

Principal Investigator: Allan Grosvenor, Ramgen Power Systems

Co- Investigators: N/A

Allocation: 40 million processors hours

Research Summary:

Ramgen Power Systems, LLC. is developing shock wave compression technology (turbomachinery operating in the supersonic relative flow regime) under an industrial partnership with Dresser Rand. The goal is to reduce the cost of Carbon Dioxide compression for carbon capture and sequestration (CCS) and to develop an engine to operate in the range of 500 kilowatts to 50 megawatts for applications such as generating electricity, running on dilute methane produced from coal mining operations, and for load leveling of solar and wind energy plants.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Exploring the Nature of the Lightest Massive Particles in the Universe.

Principal Investigator: Katrin Heitmann, ANL

Co- Investigators: Andreas Adelmann (PSI), Sudeep Das (ANL), Hal Finkel (ANL), Salman Habib (ANL), Zarija Lukic (LBNL), and Adrian Pope (ANL)

Allocation: 10 million processors hours

Research Summary:

The lightest known massive particle in the Universe, the neutrino, is the focus of major terrestrial experiments as part of the DOE Office of High Energy Physics Intensity Frontier program. The physics of the neutrino sector is also being probed by ongoing and upcoming cosmological surveys such as the Atacama Cosmology Telescope, the South Pole Telescope, and the Dark Energy Survey. The neutrino continues to surprise physicists. Introduced as a massless particle in the Standard Model of particle physics, the discovery of neutrino oscillations and therefore neutrino masses has been one of the major discoveries pointing to the existence of physics beyond the Standard Model of particle physics. Cosmological measurements of the cosmic microwave background and of large scale structure in the Universe offer a unique handle on the absolute neutrino mass and the number of neutrino species. The interpretation of these measurements hinges on large simulations that can provide accurate predictions for cosmological observables. The very light mass of the neutrinos makes such simulations very challenging: in order to enable accurate computations that can capture the effects of massive neutrinos, N-body simulations with hundreds of billions of particles have to be carried out. We will carry out large scale structure simulations using a fully self-consistent treatment of neutrinos with realistic masses for the first time. We will target the gravitational lensing of the cosmic microwave background and large scale structure probes to quantify the effect of massive neutrinos on cosmological observations.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Gyrokinetic Simulations of Multiscale Electro Turbulence for Improved Predictive Modeling of Tokamak Plasmas.

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

Co- Investigators: D.R. Mikkelsen (PPPL) and W. Guttenfelder (PPPL)

Allocation: 30 million processors hours

Research Summary:

In tokamaks (the leading approach to magnetic confinement based fusion devices), the turbulent transport of mass and energy by small-scale drift-wave microturbulence is a primary determinant of the level of confinement achieved. It is therefore essential that we be able to predict this transport with confidence in burning plasma regimes. Some of the most important open questions for predicting turbulent transport in tokamaks lie within the area of electron particle and thermal transport, which can span a significantly larger range of spatio-temporal scales than ion transport due to the smallness of the electron gyroradius relative to the ion gyroradius. Predictions of this multiscale transport with sufficient accuracy and fidelity to be robustly validated against measurements (with the full range of uncertainty quantification such comparisons entail) can only be made using the largest massively parallel systems. We propose to carry out the first systematic validation studies of multiscale electron transport for tokamak plasmas, utilizing data from the three largest US tokamak experiments. The research will exploit the unique capabilities of each device to answer the following questions:

1. What role does electron scale turbulence play in the conditions and parameters characteristic of high confinement (H-mode) tokamak operation? Does its importance depend upon the externally applied heating, and the levels of ion-scale turbulence?

2. Can the magnitude of the electron density profile “peaking” observed in current experiments be accurately predicted, and are the observed trends of this peaking with collisionality accurately reproduced? Is there an isotope dependence for the density peaking of the majority ion species? How much radial resolution is needed to capture the majority of the particle flux?

3. Can the transport driven by magnetic turbulence in high beta plasmas accurately predicted, and under what conditions do these modes play an important role?

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: HPC Colony: Adaptive System Software for Improved Resiliency and Performance.

Principal Investigator: Terry Jones, ORNL

Co- Investigators: Laxmikant (University of Illinois) and Jose Moreira (IBM)

Allocation: 6 million processors hours

Research Summary:

Operating and runtime systems provide mechanisms to manage system hardware and software resources for the efficient execution of scientific applications. By the end of this decade, exascale computers with unprecedented processor counts and complexity will require significant new levels of scalability and fault management. A significant issue arises when the system software designed decades ago for single-user use is stretched into the new needs for parallel applications running on machines consisting of hundreds of thousands of cores. The added complexity and magnitude of tomorrow's architectures restrict scalable and portable programs to only those programmers with advanced skills and detailed knowledge of today's leadership class machines. Significant improvements are required to enable a "broader application set". Our approach adapts the operating systems to the needs of applications rather than having applications constantly retooled for tomorrow's leadership class machines. Through allowing a sophisticated system software stack address performance issues, load balancing issues, and fault resilience issues, we remove these ever evolving burdens from the applications developer. Without adaptive system software, the difficulty of reaching full-machine simulations will restrict the number of teams capable of fully utilizing leadership class machines

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Computational high throughput screening of organic materials for solar energy and lighting.

Principal Investigator: Abdelkader Kara, University of Central Florida

Co- Investigators: N/A

Allocation: 6 million processors hours

Research Summary:

Understanding the interface electronic structure characteristics between organic molecules and the transition metal surfaces with different structural (degree of corrugation and bonding environment) and chemical characteristics is crucial for the design of high performance organic devices. The computational high-throughput screening of the interface characteristics involving variety of surfaces can provide the fundamental understanding and predictions for the design of the breakthrough devices with the desired highest performances. We propose to use first-principles calculations to screen the electronic structure characteristics of the interfaces between the relevant organic molecules (acenes) and eleven transition metal surfaces with different chemical identities and orientations (three surfaces). Following these computationally intensive calculations, we will further screen the electronic structure characteristics of these interfaces with the inclusion of dispersion forces through chosen implemented van der Waals corrections. The proposed research is centered on building the accurate database for screening the organic molecule-metal candidates for high performance devices. Such accurate large database will provide the ability to build descriptors for the adsorption and transport characteristics of the organic molecules on these metal surfaces, and their correlations to the thin film growth of organic materials. The proposed work is ultimately targeting the growth of efficient organic materials that are of interest to both solar energy and solid state lighting as these materials tend to be amenable to have both functionalities.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Transforming Modeling and Simulation for Nuclear Energy Applications.

Principal Investigator: Douglas Kothe, ORNL

Co- Investigators: Thomas Evan (ORNL), Mark Christon (LANL), Roger Pawlowski (SNL), and Derek Gaston, Idaho National Laboratory (INL)

Allocation: 15 million processors hours

Research Summary:

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is the Department of Energy Energy Innovation Hub established in for the modeling And simulation (M&S) of nuclear reactors (www.casl.gov). CASL applies existing M&S capabilities And develops advanced capabilities to create an environment for predictive simulation of Light Water Reactors (LWRs). This environment, the Virtual Environment for Reactor Applications (VERA), incorporates science-based models, State-of-the-art numerical methods, modern computational science and Engineering practices, and Uncertainty Quantification (UQ) and validation against Data from operating Pressurized Water Reactors, single-effect experiments, and integral tests. CASL develops and applies models, methods, data, and understanding to address three areas of Nuclear Power Plant (NPPs) performance: reducing capital and operating costs by enabling power uprates and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new NPPs; reducing nuclear waste volume generated by enabling higher fuel burnup, and enhancing nuclear safety by enabling high-fidelity predictive capability for component performance through the onset of failure. The CASL vision is to *predict with confidence, 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.* Emphasis will be coupled simulations using multiple VERA components and some single-physics analysis for model development, Sensitivity and UQ, and convergence studies.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: High level studies of excited states in light harvesting systems and complex emergent phenomena.

Principal Investigator: Karol Kowalski, Pacific Northwest National Laboratory (PNNL)

Co- Investigators: Sriram Krishnamoorthy (PNNL) and Edoardo Apra (PNNL)

Allocation: 5 million processors hours

Research Summary:

There is a general consensus that electronic structure theory needs to become reliable and predictive. This has also been echoed in a recent BES report, namely that *"without theory as a guide, the true nature of these systems(processes) may remain hidden or perhaps even be misrepresented"* and *"new theoretical concepts not only play a fundamental role in explaining existing data, but they also are instrumental in suggesting novel experiments that probe unexplored phenomena."* The central science theme of this research is to harness state-of-the-art theoretical formalisms to understand the role of electron correlation effects in designing efficient solar energy conversion light harvesting systems. The simulation effort will be targeted towards elucidating the fundamental nature of the electronic excitations and related excited-state processes in materials relevant for sustainable energy production and storage, a step essential towards advancing the clean energy agenda. These investigations will lead to understand and design new theoretical excited-state models for classes of light harvesting systems including: (1) non-covalently interacting organic molecules utilized in organic photovoltaic devices, (2) aryl and malonic acid functionalized forms of the porphyrins, (3) molecular graphenes and (4) carotenoids.. With ongoing development of scalable high-order methods, some of the requested computer time will also be used for development and testing at scale new capabilities as they become available. The proposed calculations will aim to reach a scale never approached before and feasible only with recent advances in theory, software, and hardware.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Massively Parallel High Fidelity Simulation of Spray Atomization.

Principal Investigator: Xiaoyi Li, United Technologies Research Center

Co- Investigators: Marios Soteriou (United Technologies Research Center)

Allocation: 20 million processors hours

Research Summary:

The atomization of fuel jets by aerodynamic forces, as the first step in the overall spray combustion process, is highly critical for the performance of many commercial and military aerospace applications such as gas turbine combustors, afterburners, scramjets and ramjets. Understanding the complicated multiphase flow with liquid breaking/merging occurring in a wide range of scales poses a grand challenge to the scientific community. As a result, fuel atomization has been the subject of substantial research efforts in the past. Despite these efforts, limited understanding of the details of this complex multiphase flow has been achieved with concomitant severe limitations in ability to predict atomization behavior and effectively impact design. This is due to the inherent complexity of the physical phenomena involved which impose severe limitations on experimental measurement (e.g. lack of optical accessibility) and which have challenged ability for detailed simulation due to unavailability of models and severe computational cost requirements. Recent advances in spray atomization modeling together with the outstanding growth in computational methodology and capability, however, have been relaxing these limitations to the point that for the first time, first principle simulations of spray atomization are becoming feasible on massively parallel computers. *It is the objective of this research to demonstrate this feasibility by coupling advanced, modern algorithms with the state-of-the-art with high performance computing hardware*. The expectation is that such simulations will also advance current scientific understanding and will potentially impact product design in the future In the past two years, success has been achieved in developing a first-principle multiphase flow solver validating its solution against experimental data and improving its scalability to intermediate scales. However, the computational size is limited to the range that can resolve length scales that are still much larger than the ones encountered in realistic aerospace applications. A simulation case of cm size domain with grid cells resolving down to 40 μm requires several thousand processors running for two weeks, consuming millions of CPU hours. Merely doubling the grid resolution would require 16 times more computing resources (due to refinement in 3 spatial and 1 temporal dimensions). Utilization of Adaptive Mesh Refinement (AMR) can partially overcome the difficulty of cost increase, but currently such algorithms still suffer from unsatisfactory scalability of performance. The research aims to scale up our simulation capability by further improving the scalability of our AMR-based solver and utilizing hybrid programming methodologies that are best tuned to the underlying heterogeneous computing architecture involving multi-core processors and GPU accelerators. A number of cases simulating spray atomization at high-shear operating conditions will be performed using the accelerated solver. The simulation results will be used to develop fundamental understanding of the underlying physical processes and to demonstrate the potential of using HPC simulations to impact industrial design.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Gyrokinetic Simulation of Energetic Particle Turbulence and Transport.

Principal Investigator: Zhihong Lin, University of California, Irvine

Co- Investigators: N/A

Allocation: 20 million processors hours

Research Summary:

This award will study the confinement of energetic particles in fusion plasmas. To accurately predict The confinement properties of energetic particles in burning plasmas, the simulations must incorporate kinetic effects of thermal and energetic particles and nonlinear interactions of turbulence. This award will study new physics in the energetic particle turbulence and transport, including the kinetic effects of thermal particles on energetic particle instability, the transport of energetic particles, and turbulence. The goal is to build the predictive capability for energetic particle turbulence and transport in the ITER burning plasmas, which requires understanding nonlinear physics of energetic particle instability, predicting energetic particle transport given a fixed energetic particle drive, and self-consistent simulations of a full cycle of the energetic particle turbulence. These are the critical next steps for building the predictive capability of energetic particle confinement in ITER.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Predictive simulations of cuprate high-temperature superconductors.

Principal Investigator: Thomas Maier, ORNL

Co- Investigators: Thomas Schulthess, ETH Zurich

Allocation: 50 million processors hours

Research Summary:

We will conduct the first ever systematic and fully ab-initio many-body simulations of cuprate high-temperature superconductors using combinations of state-of-the-art electronic structure and quantum many-body techniques and codes that have proven to run and scale efficiently. Understanding the mechanism that leads to superconductivity in these systems and the factors that determine the large variation of transition temperatures is one of the grand challenges of condensed matter physics and will be our primary goal. With the availability of petascale supercomputers and the growing sophistication of quantum simulation methods, we are now in a position to extend the frontiers to solve these questions and make important progress in the field. Cuprate high-temperature superconductors are among the most challenging systems in condensed matter physics. Traditional electronic structure approaches generally fail to describe their physics, which is driven by the effects of strong electronic interactions. Combinations of density functional theory-based approaches and many-body theory are the generally accepted strategy for computing from first-principles the electronic structure of correlated systems. We will calculate trends in the superconducting transition temperatures among different cuprate compounds. The prediction of the extreme case factor 5 difference in transition temperature is a great challenge, but if successful, will allow us to obtain a detailed understanding of the factors that determine *T*c in these systems.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Petascale Thermal Hydraulic Simulations in support of CESAR.

Principal Investigator: Elia Merzari, ANL

Co- Investigators: Paul Fischer (ANL), Justin Walker (ANL), and Andrew Siegel (ANL)

Allocation: 30 million processors hours

Research Summary:

The Center for Exascale Simulation for Advanced Reactors (CESAR) aims to develop a coupled, next generation nuclear reactor core simulation tool capable of efficient execution on exascale computing platforms. This center helps fulfill the mission of the Advanced Scientific Computing Research (ASCR) program which is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE). In fact a particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science.

In support of the mission of CESAR, large petascale-level simulations are needed to address the limitations of current methods and address the potential scaling to larger machines. This proposal focuses on the thermal-hydraulic part of CESAR and in particular to the following problems:

1. A high-fidelity simulation using the large eddy simulation (LES) model of the Multi-Application Small Light Water Reactor (MASLWR) experiment, which is a facility in SCALE with the current Nuscale Reactor design. The data and scaling information obtained will provide insight into the challenges exascale simulations will face. This simulation will also help providing useful guidance in the startup analysis of the reactor.
2. A full high fidelity LES simulation of a 37-rod bundle. The core of nuclear reactors is arranged in rod bundles and the coolant flow outside them is complex and still a matter of research. This data will be used to examine in detail rod-bundle flows at a level never achieved before and help determine computational cost in the exascale limit.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Coupled electronic and nuclear dynamics in solar photocatalytic water splitting.

Principal Investigator: Thomas Miller, California Institute of Technology

Co- Investigators: N/A

Allocation: 22 million processors hours

Research Summary:

We will employ massively parallel quantum dynamics methods to advance the understanding of the conversion of solar energy to molecular fuels. Computational research has the potential to contribute in this area by allowing for detailed investigations of biological photosystems, by revealing key insights into fundamental photochemical processes, and by allowing for fast and inexpensive screening of candidate photosystems. We have developed massively parallelizable theoretical methods that overcome the intrinsic challenges of simulating and understanding the dynamics of processes that are central to solar photocatalysis. With leadership-scale computational resources, we will use these new methods to elucidate the chemical reaction dynamics at the heart of organometallic catalysts and the photocatalytic water splitting pathway of Photosystem II. The proposed research will yield fundamental insights into natural photosynthesis, as well as new strategies for the design of biomimetic photocatalysts.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Prediction of Multiscale, Multiphysics Turbulent Flow Phenomena Using Unstructured Large Eddy Simulation.

Principal Investigator: Parviz Moin, Stanford University

Co- Investigators: N/A

Allocation: 80 million processors hours

Research Summary:

This project aims to broaden the community of researchers able to fully utilize leadership computing resources to predict and quantify the uncertainty of multiscale, multiphysics turbulent flow phenomena using the one-of-its-kind, exascale-ready unstructured large-eddy simulation (LES) platform, CharLES. We will support three projects: LES of supersonic jet noise “crackle” in complex geometry nozzles, LES of supersonic combustion with finite-rate chemistry in turbulent mixing layers, and an explicitly filtered LES of a three-dimensional stalled diffuser to verify grid-independence.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: U.S.-Russia Collaboration on Verification and Validation in Thermal Hydraulics: Nek5000 and Conv3D Simulation of "SIBERIA" Experiment.

Principal Investigator: Aleksandr Obabko, ANL

Co- Investigators: Paul Fischer (ANL), W. David Pointer (ANL), Vladimir V. Chudanov (Moscow Institute of Nuclear Energy Safety), Valeriy A. Pervichko (Moscow Institute of Nuclear Energy Safety), and Anton A. Kanaev (Moscow Institute of Nuclear Energy Safety)

Allocation: 30 million processor hours

Research Summary:

Safer nuclear energy power promises to become a reliable, carbon-free resource capable of meeting a 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 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 to analyze, model, simulate, and predict complex thermo-fluid phenomena will help advance nuclear power capabilities by resolving technical, cost, and safety issues.

One of the critical safety parameters in a nuclear power plant is the peak material temperature, which must be maintained well below the melting point of the core structural components such as the cladding, fuel, and subassembly walls. Prediction of the peak temperature, as well as the associated uncertainty, involves in part an accurate computation of thermal mixing governed by thermal conduction and convection in a complex geometry. The higher-fidelity thermal hydraulics codes will help simulate nuclear systems with well-defined and validated prediction capabilities.

Two thermal hydraulics codes we will cross-verify and validate in this project are Argonne National Laboratory's highly scalable, open-source spectral-element code Nek5000 and the Conv3D code developed at the Moscow Institute of Nuclear Energy Safety (IBRAE). As part of an international engagement mandated by DOE in support of the safe, secure, and peaceful use of nuclear energy, we have initiated a collaborative activity between Argonne and IBRAE that involves the cross-verification and validation of the LES simulations by Nek5000 and Conv3D codes based on the experimental setup of "SIBIERIA." The advantage of this concurrent experiment in Novosibirsk, Russia is the capability of high-precision, time-dependent measurements of near-wall flow with a novel electro-diffusion method that makes "SIBIERIA" particularly suitable for validation of high-fidelity computational fluid dynamics codes.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Ab Initio Hyper-Nuclear Physics.

Principal Investigator: Konstantinos Orginos, College of William and Mary

Co- Investigators: Silas Beane (University of New Hampshire), Emmanuel Chang (University of Barcelona), Saul Cohen (University of Washington), William Detmold (College of William and Mary), Robert Edwards (Jefferson Laboratory), Balint Joo (Jefferson Laboratory), Huey-Wen Lin (University of Washington), Thomas Luu (Lawrence Livermore National Laboratory), Parikshit Junnarjar (University of New Hampshire), Stefan Meinel (College of William and Mary), Assumpta Parreno (University of Barcelona), David Richards (Jefferson Laboratory), Martin Savage (University of Washington), and Andre Walker-Loud (College of William and Mary)

Allocation: 70 million processors hours

Research Summary:

We will implement an ab initio study of nuclear physics. The overall goal of this project is to study the spectrum of light nuclei and hypernuclei directly from the underlying quantum field theory of the strong interactions, quantum chromodynamics (QCD). This is a central goal of nuclear physics research, impacting the worldwide hypernuclear experimental program, as well as nuclear astrophysics, where it will refine our understanding of stellar evolution and core collapse. Our three part proposal will A) obtain the spectrum of light nuclei and hypernuclei directly from QCD at unphysically large quark masses, B) provide the first physical predictions of this spectrum, and, finally, C) calculate this spectrum with dynamical up, down and strange quarks with their physical masses. Successful completion of this plan will firmly establish the foundational basis of nuclear physics in the Standard Model, and provide an exploration of a new frontier in nuclear science.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Dynamics of conformational transition in thermo-sensitive polymers and hydrogels.

Principal Investigator: Subramanian Sankaranarayanan, ANL

Co- Investigators: Sanket Deshmukh (ANL) and Derrick Mancini (ANL)

Allocation: 50 million processors hours

Research Summary:

Understanding the conformational transformations of isolated linear polymer chains and their macromolecular architectures is a fundamental problem in the field of polymer science. Altering environmental variables such as temperature, pH, light, or providing external stimuli such as magnetic and electric fields can bring about these conformational changes. Thermo-sensitive polymers such as poly(n-isopropylacrylamide) (PNIPAM) represent an important class of materials, which undergo coil-to-globule transition across the lower critical solution temperature (LCST), which is around 305K. These coil-to-globule transitions are of importance in a number of practical applications including drug delivery, medical diagnostics, tissue engineering, electrophoresis, separation, and enhanced oil recovery to name a few. For example, tuning the LCST of PNIPAM close to human body temperature *via* copolymerization can enable development of controlled drug delivery system. Atomic scale mechanism of the coil-to-globule collapse is not very well known and knowledge about this collapse might be useful in designing novel materials with well defined LCST characteristics. Given that the link between specific molecular (microscopic) and macroscopic properties is still not clearly understood, tuning the conformational transition through the LCST represents a significant challenge. We develop strategies to tune these conformational transformations occurring at the atomic scale for polymers ranging from single chain oligomers to their macromolecular architectures. The first involves polymerization with different co-monomers and addition of different additives to alter the LCST and allow us to control the functional properties of the polymer. We will evaluate the effects of copolymerization of PNIPAM and poly (ethylene glycol) (PEG) (also known as poly(ethylene oxide) (PEO) on the resulting atomic scale s using molecular dynamics (MD) simulations. Hydrophilic monomers elevate the LCST while copolymerization with hydrophobic monomers depresses the LCST.Hydrophilic monomers, such as PEG have the LCST around 80 to 100 °C, based on its molecular weight, and keeps polymer solvated above 305K. This could result in an increase in the LCST of PNIPAM. Atomistic simulations will be used to evaluate the copolymerization effects arising from various hydrophilic and hydrophobic monomers. Other strategies involve altering the LCST of PNIPAM by adding salts to perturb the ionic concentration or by adding solvents such as methanol or ethanol in water to alter hydrogen-bonding characteristics of polymer-solvent. While it is known that addition of salt such as Na+Cl- reduces LCST, the exact origin and mechanism of lowering of the LCST is still unanswered. Atomic scale insights on the ion-water, and ion-polymer structures using MD simulations will be useful for tuning the LCST. In the presence of methanol, LCST of PNIPAM is depressed and it is speculated that addition of methanol affects the PNIPAM-water interactions. However, the atomic scale PNIPAM-methanol and methanol-water interaction are not completely understood. We therefore propose to use MD simulations to investigate the effect of solvent mixed with salt or methanol on conformational transformations and the LCST of PNIPAM. The atomic trajectories obtained from MD simulations will also be used to study the various polymer-solvent interactions and solvation dynamics of surrounding media and its role in inducing changes at the atomistic level. These studies will subsequently be extended to macromolecular architectures such as polymer brushes and gels of PNIPAM. Results from these simulations will be compared with the ongoing experiments being carried out at the APS division at ANL.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Validation work for heterogeneous nuclear reactor calculations.

Principal Investigator: Micheal Smith, ANL

Co- Investigators: D. Kaushik (ANL), A. Marin-Lafleche (ANL), A. Mohamed (ANL), C. H. Lee (ANL) and E. Wolters (ANL)

Allocation: 30 million processor hours

Research Summary:

The goal of the Simulation based High-efficiency Advanced Reactor Prototyping (SHARP) project at Argonne National Laboratory is to enhance the state-of-the-art nuclear reactor core modeling capabilities in the context of assessing their ability to better solve real-world design problems. The SHARP project is primarily supported by DOE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program but has additional support from the Center for Exascale Simulation for Advanced Reactors (CESAR). The goal of NEAMS is to develop new tools that push the envelope of nuclear reactor analysis while CESAR is focused on co-designing the fundamental algorithms and super-computers such that simulation codes like SHARP can progress with technology. NEAMS has two foci: (1) the enhancement of newly developed high-fidelity simulation methods in preparation for design analysis, and (2) the application of the advanced methods to core problems for an accurate assessment of key system performance and safety characteristics in nuclear reactors.

Code development requires substantial verification and validation work before confidence in its use is justified. Up to now, the majority of the UNIC code validation work has been done using well-understood methodologies involving spatial homogenization. From this point forward, a more substantial number of verification and validation problems will be tackled. Efforts will focus on solving the Flattop and spherical problems Godiva and Jezebel and on addressing an outstanding request from Idaho National Laboratory to demonstrate the ability of the UNIC code to model the Advanced Test Reactor (ATR). From a science perspective, we will improve the existing simulation capability by:

- Continued development of the cross section generation technique for homogeneous, mixed homogeneous-heterogeneous, and fully heterogeneous geometry modeling in steady-state as well as kinetics/dynamics modeling of fast reactors.

- Initial validation of the heterogeneous modeling capability of UNIC on fast and thermal reactor problems using a wider set of benchmark problems.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Reducing Uncertainty of Climate Simulations Using the Super-Parameterization.

Principal Investigator: Christiana Stan, George Mason University

Co- Investigators: N/A

Allocation: 11 million processors hours

Research Summary:

The primary goal of the research is to conduct and analyze simulations in which cloud precesses are based on the "super-parameterization". The effects of moist convection, stratiform cloudiness, radiative transfer and boundary-layer processes will be computed by embedding a 2D cloud resolving model. The ultimate goal of super-parameterization is to reduce the range of uncertainty in representation of cloud processes. We will perform one simulation of the twentieth century climate and one of the twenty-first century climate based. Our analysis will focus on improving our understanding of the role of cloud processes on the critical processes and modes of variability in the earth system. The objectives of the anthropogenic climate change experiments are to answer questions like 1) Does the explicit representation of clouds change the projected global mean warming and the associated increase in global mean precipitation estimated from simulations with conventional cloud parameterizations? 2) Do patterns of change projected by the current generation of models depend on the representation of cloud processes? 3) Is El Nino interannual variability sensitive to cloud representation? 4) Does global warming in this model leads to a change in the El Nino? These experiments are unique by combining the high-resolution representation of large-scale processes with cloud-scale resolution for the representation of moist convection, stratiform clouds radiative transfer and boundary-layer processes.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: VUQ Assessment of a Large Eddy Simulation Tool for Clean-Coal Technology.

Principal Investigator: Jeremy Thornock, University of Utah

Co- Investigators: Martin Berzins (University of Utah) and John Schmidt (University of Utah)

Allocation: 20 million processors hours

Research Summary:

This research proposal is for using simulation science to explore ways to improve clean coaltechnologies for the generation of electric power. Specifically, we will use a combination of simulations using the Arches component of the Utah Uintah open source framework and experimental data provided by our industrial collaborator Alstom Power to investigate coal combustion under oxy-coal conditions including stability, variability of inlet conditions, including recycle rates and coal types and coal ignition within the boiler. The end result of these simulations is to demonstrate the predictive capabilities of large scale large eddy simulations in the design and development of industrially sized boilers. The aim is to use petascale simulations to investigate the design space required to develop more efficient oxy-coal boiler technologies We are in a unique position to deliver quantifiable and predictable technologies that will improve the design of industrially sized coal boilers. With these new boiler designs the environmental impact will be lessened by the reduction in greenhouse gas emissions while still relying on the United States most abundant natural resource.

2012 ASCR Leadership Computing Challenge (ALCC) Allocations

Title: Multiscale Modeling of CO2 Sequestration in Carboxysomes.

Principal Investigator: Gregory Voth, ANL

Co- Investigators: N/A

Allocation: 8 million processors hours

Research Summary:

Many challenges remain in the development of renewable energy technologies to fulfill the energy production and storage needs for the future of the United States. One promising paradigm involves the generation of biofuels from plant material and microorganisms via solar energy, specifically using natural photosynthesis to produce useful chemicals. Nature has provided photosynthetic bacteria with an efficient mechanism to transform atmospheric carbon dioxide (CO_2) into useful organic sugar-phosphates, which are subsequently converted into important energy-providing compounds. Inefficiencies in the enzymatic processes required to fix (transform) carbon to organic molecules are overcome by generating high concentration of CO_2 in the bacteria that are localized in a specialized microcompartment, the *carboxysome*, which sequesters both CO_2 and the enzymes crucial for the bacterial carbon conversion process. A detailed molecular-level understanding of how such organisms have optimized the carbon fixation process, which plays a crucial role in the global carbon cycle remains incomplete. The computing resources will be used to provide insight into the molecular mechanism of the carbon fixation by combining novel theory and simulation techniques in the design and implementation of an accurate multi-scale methodology that accounts for reactive dynamics, i.e. for the dynamic evolution of chemical bonds during reactive processes. Molecular-level insight will be acquired into the properties of the multi-protein carboxysome shell and important enzymes within.

The carboxysome's role in maintaining high CO_2 concentrations is key to the efficiency of the otherwise particularly slow enzymatic reactions involved in the energy conversion. Although important structural insights from experiments are elucidating the carboxysome shell structure, many questions remain regarding the formation of this shell and how it encapsulates and influences the sequestered enzymes. In order to provide a molecular level description of these complex carboxysome systems, we will use multiscale modeling of the key steps in the enzymatic fixation of carbon and the assembly of the carboxysome shell. The enzymatic reactions will be modeled using reactive molecular dynamics and the multistate empirical valence bond methodology. The results of large-scale, all-atom simulations will be used to develop coarse-grained models of the key enzymes and those proteins that compose the carboxysome shell. These two methods will subsequently be combined to develop a methodology for mixed-resolution reactive simulations. A detailed molecular-level understanding of these important systems will prove to be important not only in the design of future clean energy technologies, but will provide a significant contribution to the fields of chemistry, biology, and materials science.