**TITLE:** Understanding the factors that affect the efficiency of bio-catalytic processes


**PRINCIPAL INVESTIGATOR:** Pratul Agarwal, Oak Ridge National Laboratory
**CO- INVESTIGATOR:** Chakra Chennubhotla, University of Pittsburgh

**ABSTRACT:**
Bio-catalytic processes have implications for research related to the mission of Department of Energy (DOE) in renewable energy and carbon sequestration strategies. Naturally occurring enzymes including cellulases have been investigated for applications in large-scale degradation of cellulose to sugars, which can serve as fermentation raw material for production of low-cost bioethanol. For offsetting the environmental effects of fossil-fuel consumption, the enzyme ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO) has been investigated for applications in carbon sequestration strategies. Improvements in the efficiency of these bio-catalytic processes are required to make their usage at industrial scale cost-effective.

Computational simulations continue to provide vital insights into the mechanism of enzyme function as well as the factors that contribute to the catalytic efficiency of bio-catalytic processes. Our ongoing efforts are providing new detailed insights into the biophysical mechanism of enzyme mediated bio-catalysis. In particular, our computational investigations have revealed that enzymes are not rigid molecules but intrinsically flexible molecules with a wide range of internal motions. Special internal motions present within enzyme systems are closely linked to the mechanism of catalysis. We have discovered that these internal protein motions as well as the associated motions of the surrounding solvent enable the high catalytic efficiency of enzymes through a network of vibrations. A detailed understanding of the catalytic processes requires the detailed information about the role of various enzyme residues (near and away from the active-sites) in these enzyme networks. Moreover, it is becoming clear that the efficiency of a bio-catalytic process is related to the presence of different conformational sub-states during the catalytic pathway. The identification and quantification of these catalytically competent conformational populations are critical for understanding the efficiency of the overall process. Our computational methodology is based on the use of molecular dynamics (MD) simulations on high-performance computing (HPC) resources, such as the ones available on ORNL's JaguarPF supercomputer. HPC resources are essential for our ongoing investigations as it allows the required amount of conformational sampling and accurate free energy estimates that are central to our discoveries. Note that in the past years, access to ORNL's HPC machines has allowed us to publish eight papers (and four more in review process) in the area of proposed research.

Building upon the preliminary success, we continue to pursue theoretical & computational modeling driven investigations of bio-catalytic processes. Specifically we are focusing on:

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- Developing computational methodology for identification of conformational sub-states
- Identification of structural and conformational factors that affect the catalytic efficiency

- Applying the developed methodology to investigate cellulase Cel9A from *Thermobifida fusca* and RuBisCO from *Rhodospirillum rubrum*

We therefore request allocation on ORNL's Cray XT5. Highly scalable codes such as LAMMPS, NAMD, and PMEMD (AMBER) among others will be utilized to perform large-scale MD simulations.

**TITLE:** Petascale kinetic plasma simulation of the interaction among laser speckles in laser-driven inertial fusion energy settings

**PRINCIPAL INVESTIGATOR:** Brian Albright, Los Alamos National Laboratory (LANL)
**CO-INVESTIGATORS:** Lin Yin, LANL, Harvey Rose, LANL

**ABSTRACT:**
We propose to use the Leadership-Class supercomputing on ORNL Jaguar and our proven VPIC kinetic plasma code to conduct the first-ever systematic*, ab initio s*imulation study of laser-plasma interaction in meso-scale media, where laser speckles can couple to one another through an exchange of particles and waves. This basic physics problem is central to laser-driven inertial fusion energy, a viable approach to the DOE clean energy initiative, and is one of the "Grand Challenges" of high energy density laboratory physics, as identified by a DOE-convened panel of experts and reported in a recent DOE Office of Science report [*Rosner and Hammer, 2009*]. Understanding the nature of nonlinear, emergent coupling among laser speckles, or bright spots in laser beams, requires computing resources that have only recently become available with the advent of petaflop/s supercomputing. The culmination of this work will be an improved understanding of the essential nature of laser-plasma interaction that can be used to guide the design of future laser-driven inertial fusion energy experiments and help assess the viability of laser-driven inertial fusion energy as a clean energy concept.

**TITLE:** Reliable Predication of Performance of High Lift Systems of Commercial Aircraft

**PRINCIPAL INVESTIGATOR:** John Bussoletti, Boeing

**ABSTRACT:**
Current methods for designing and analyzing commercial aircraft in take-off and landing configurations (high lift configurations) rely heavily on wind tunnel tests. These costly tests can take months of flow time to perform, and include the building of very complicated wind tunnel models. Running at realistic Reynolds numbers is a prohibitively expensive proposition (requiring the use of cryogenic wind tunnels with their attendant issues). Therefore, most models are tested in the wind tunnels at lower Reynolds numbers and the results are built up to full scale based on experience. If we could accurately and quickly compute such cases using Computational Fluid Dynamics (CFD), especially at full scale Reynolds numbers, it would give us a tremendous advantage in cycle time, cost and airplane performance. The grand challenge problem in CFD is the prediction of the maximum lift coefficient (CLmax) and especially its variation with respect to Reynolds number and various configuration parameters, such as chord lengths of elements and their positioning. There is substantial evidence that the accuracy of the prediction of CLmax is sensitive to both solution accuracy (residual convergence) and grid characteristics. Thus to obtain meaningful estimates for CLmax, the simulations should be residual-converged and grid-converged.

Over the course of year 2010, access to ORNL computing facilities under the INCITE program has enabled us to test and verify the accuracy, scalability, sensitivity to grid density and robustness of a code to assess aircraft performance in take-off and landing configurations. In particular, the Cray XT-5 computer (Jaguar) with 16GB of memory and 12 cores per compute node, has enabled us to carry out CFD simulations using up to 50 million grid points using only a small fraction of the total system resources. These are extremely challenging cases to compute, since the geometries are complex and the flow fields are complicated featuring significant flow phenomena such as smooth body separation, interactions between shear layers, wakes and boundary layers and possibly even shocks (even though the aircraft flies at low speeds). In addition, in this flow regime, it is well known that hysteresis effects are encountered experimentally. In our work under the INCITE program we were also able to demonstrate the existence of hysteresis effects in our computational model, and even discovered the existence of three independent solutions, all converged to machine zero on the same grid, at the same flight condition by simply modifying the initial state of the solution vector.

For the current year, the scope of our effort is focused on low speed (high lift) modeling issues and "steady state" solutions to the Reynolds-Averaged Navier-Stokes equations with the Spalart-Allmaras turbulence model. In the future, our efforts will expand to consider the benefits of additional physical modeling extensions such as Detached Eddy Simulation and Unsteady RANS simulations as well as an expansion into other flow regimes such as transonic cruise and buffet onset conditions at transonic flow conditions.

At Boeing, we have developed a two-dimensional analysis capability called GGNS2D (Reference 1) which is used widely within the company for analysis of two-dimensional high lift configurations. GGNS2D:

- Takes an analytic description of the geometry and flow conditions as inputs

- Uses a robust globalized Newton's method as the nonlinear solver
- Uses a direct sparse factorization as the linear solver
- Employs solution adaptive gridding that automatically places grid points in regions of interest and aligns the grid edges to conform to the flow

This is a unique analysis capability and has been incorporated into the design process as well. We are currently in the process of developing a similar capability in three dimensions.

Under an INCITE project in 2010, we have tested our 3D solver on a sequence of fixed grids (of increasing sizes) for the AIAA "Trap Wing" configuration (Reference 2). We have had encouraging results in terms of the accuracy of our predictions, compared to other available codes. In addition the INCITE grant provided the opportunity to test the scalability of our new code, (the relationship between the time necessary to run the code to the number of computer processors it uses). We have found that our code scales extremely well, scaling nearly linearly. We have recently demonstrated the ability to run our code analyzing a takeoff configuration in as little as two hours. When fully validated, such a capability could allow us to make radical changes to our wing design process. To date, most of our runs at ORNL have been with fixed grids (wherein one generates an unstructured grid about the complex configuration using rules of thumb for grid distribution). While this has enabled us to confirm that the solver technology does hold up when solving large problems (up to 50 million vertices or 300 million degrees of freedom), we would like to continue to develop the adaptive grid capability in three dimensions. We believe that developing this capability will help us address the grand challenge problem of the prediction of CLmax as a function of various configuration parameters and Reynolds number.

**TITLE:** Toward Crystal Engineering from First Principles

**PRINCIPAL INVESTIGATOR:** James R. Chelikowsky, University of Texas at Austin
**CO-INVESTIGATORS:** Noa Marom, University of Texas at Austin
Jeff R. Hammond, Argonne National Laboratory
O Anatole von Lilienfeld, Argonne National Laboratory
Alexandre Tkatchenko, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg, Germany

**ABSTRACT:**
Crystal engineering is a bottom-up approach to designing new crystalline materials out of molecular building blocks with vast and far-reaching applications. It is fascinating that seemingly unrelated applications, such as developing antimalarial drugs and developing metal-organic frameworks (MOFs) for hydrogen storage, share similar design principles and synthesis strategies.

We seek a deeper understanding of the intermolecular interactions that govern the properties and synthesis of supramolecular entities in order to enable computational crystal engineering from first principles. For this purpose, we will employ density functional theory (DFT) in conjunction with the Tkatchenko-Scheffler van der Waals correction (TS-vdW). We will focus primarily on demonstrating the capability of our approach to describe correctly the geometry, electronic structure, and energetics of known supramolecular systems. This will be done through a series of case studies exemplifying generally applicable concepts in crystal engineering, namely, the prediction of polymorphism in molecular crystals, the interaction of hydrogen with MOFs, and the control of crystallization by tailor-made additives. The case studies will be chosen to reflect the wide variety of applications of crystal engineering from biological systems, such as amino acids and antimalarial drugs, to technological applications, such as dye-sensitized TiO2 clusters for solar cells and MOFs for hydrogen storage. The systems we intend to study comprise several hundred atoms, pushing the size limits of fully quantum mechanical electronic structure calculations and requiring massively parallel computing.

**TITLE:** Fundamental combustion simulations to enable clean energy breakthroughs in low-carbon gas-turbine combustion systems

**PRINCIPAL INVESTIGATOR:** Jacqueline H. Chen Sandia National Laboratories (SNL)
**CO-INVESTIGATORS:** Hemanth N. Kolla, SNL,
Ray W. Grout, National Renewable Energy Laboratory
Evatt R. Hawkes, The University of New South Wales
Andrea Gruber, SINTEF Energy Research

**ABSTRACT:**
We propose to perform first principles direct numerical simulation focusing on science underpinning efficient power generation via gas-turbine combined cycles, potentially coupled with carbon-capture and storage, which minimizes net carbon emissions as well as locally harmful pollutants such as NOx. In this context, alternative low-carbon fuels (*i.e.* hydrogen-rich) are of great interest to gas turbine manufacturers. However, enormous challenges must be overcome in order to achieve efficient and clean combustion of these fuels in modern gas turbines.

The challenges associated with these fuels can be traced to their differing reactivity, mixing and diffusion characteristics compared to traditional hydrocarbons, leading to dramatically different combustion behavior. In consultation with key players in the gas turbine industry, *e.g.* GE, Alstom Power, and SINTEF, we have identified a set of keystone direct numerical simulation target problems that will address one of the foremost design challenges for gas turbine combustors operating with low-carbon fuels, the efficient and safe fuel injection that allows rapid transition to (ultra) lean conditions. By systematically varying the fuel composition for this keystone target, the DNS will provide fundamental insight into the mechanisms of flame anchoring, stabilization, and propagation for premixed and non-premixed jet flames in cross-flowing configurations. These basic issues are crucial to the development of gas turbines operating with hydrogen-rich fuels and must be addressed at a fundamental level. The DNS will also provide unique scientifically grounded validation data for the development of full-scale models of gas turbines.

**TITLE:** Projections of Ice Sheet Evolution Using Advanced Ice and Ocean Models

**PRINCIPAL INVESTIGATOR:** William D. Collins**,** Lawrence Berkeley National Laboratory (LBNL)
**CO-INVESTIGATORS:**
Daniel F. Martin, LBNL
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**ABSTRACT:**
The Greenland and Antarctic ice sheets are making a significant and growing contribution to global sea-level rise. As the climate continues to change, there is a risk of abrupt retreat of marine-based ice sheets in contact with a warming ocean. 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. These simulations would leverage several recent DOE-funded advances in ice-sheet and ocean modeling. 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 a scalable, higher-order ice sheet model with adaptive mesh refinement (AMR). LANL scientists have developed novel methods for simulating ocean circulation and heat exchange beneath advancing and retreating ice shelves. Also, a LANL-led effort has resulted in the inclusion of an active ice sheet model in the Community Earth System Model (CESM). 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-owing regions, where dynamical length scales are O (1 km) or less.

We request ALCC computing resources to conduct pathbreaking simulations of decade-to-century-scale ice-sheet evolution. We will carry out three kinds of simulations: (1) standalone ice-sheet simulations with the new AMR model, (2) ocean simulations with a modified version of the POP model that allows dynamic interactions with ice shelves, and (3) coupled ice-sheet/ocean simulations at regional to global scales. These simulations will constitute an important contribution to ice-sheet and sea-level projections in the Fifth Assessment Report (AR5) of the Intergovernmental Panel on Climate Change (IPCC). Findings and output from the simulations will be shared with the IPCC author team and the broader glaciology and climate modeling communities.

**TITLE:** First Principles Calculations of Interfaces in Electrical Energy Storage Systems

**PRINCIPAL INVESTIGATOR:** Larry A. Curtiss, Argonne National Laboratory (ANL)

**CO-INVESTIGATORS:** Jeffrey Greeley, ANL
Hakim Iddir, ANL
Peter Zapol, ANL

**ABSTRACT:**
The design and discovery of new materials are crucial to our energy future. Massively parallel quantum chemical calculations will play a crucial role in the design of breakthrough materials to help make the advances needed. In this proposal, we detail how we will utilize an allocation of time on the ANL Blue Gene/P facility to provide the fundamental understanding and predictions needed to understand and design new materials for electrical energy storage. We will use new electronic structure codes that are becoming available for running on massively parallel computer clusters in combination with new concepts in materials design and synergies with world-leading experimental groups in battery research.

We propose to use massively parallel computing to model the physical/chemical complexities of electrolyte reactions and growth of interfaces in lithium-ion and other types of batteries from first-principles calculations that has not been possible before and to use this information to help develop new materials that can extend the lifetime and safety of batteries. There has been much progress in the development of electronic structure codes capable of running in parallel on tens of thousands of computational cores. Among these are the GPAW code, which is a grid-based density functional theory code pioneered by Jens Nørskov's group in Denmark, who have teamed up with Argonne researchers in the Center for Nanoscale Materials (CNM) and Argonne Leadership Computing Facility (ALCF) to adapt these codes for use on the Blue Gene/P. The ALCC allocation requested in this proposal will be focused on several aspects of materials development of lithium ion batteries. The first is modeling of the growth and properties of the solid-electrolyte interphase (SEI) from electrolyte additives and the second is on new coating materials for the anode itself. This will have practical applications such as safer lithium ion batteries for electric vehicles and new battery technologies for longer range electric vehicles**.**

**TITLE:** The interactions between vaporizing liquid droplets and a turbulent flow: Fully resolved direct numerical simulation

**PRINCIPAL INVESTIGATOR:** Said Elghobashi, University of California, Irvine

**ABSTRACT:**
The objective of the proposed numerical study is to enhance the understanding of liquid droplet vaporization and mixing processes in a turbulent flow. The numerical study employs direct numerical simulations (DNS) to examine the two-way interactions between freely-moving vaporizing droplets and isotropic turbulence. The droplets will be *fully resolved* in 3D space and time, i.e. not treated as point particles, and all the scales of the turbulent motion are resolved down to the smallest relevant length- and time-scales (the Kolmogorov scales). The emphasis will be on the two-way exchange of mass, momentum and energy between the vaporizing droplets and the surrounding turbulent gas. The turbulence will be assumed isotropic as a first step before considering turbulent shear flows in future studies.

The proposed DNS study will be the *first* that fully resolves the flow inside and outside a large number of freely-moving vaporizing droplets in a turbulent flow. The detailed results of the proposed DNS, with two-way coupling between the droplets and turbulence, can be used to develop and verify the mathematical models for the subgrid scales of large eddy simulations (LES) as well as Reynolds-averaged models. It should be emphasized that the detailed DNS data which will be obtained from the proposed research are not available in any published experimental or numerical study (Birouk & Gokalp, 2006).

The experimental study which is being currently performed in parallel with the DNS study will examine the effects of turbulence on the vaporization rate of a single droplet moving freely in isotropic turbulence. In addition to enhancing the understanding of the physics of interaction between turbulence and vaporization, the measurements will be used to validate our DNS methodology since no other comparable experimental data exist for free-flying droplet evaporation in isotropic turbulence where the Kolmogorov length scale of turbulence is smaller than the initial droplet size. Hence, the coupled experiment and computations will determine the key interactions between evaporation and turbulence.

The results of the proposed study will have a significant impact on the efficient utilization of energy. This impact stems from the fact that the vaporization rate is the main controlling mechanism of fuel droplet combustion and that liquid fuels are the most important source of energy for all modes of transportation and will remain as such for the foreseeable future. Understanding the physical details of the vaporization and mixing processes in a turbulent flow is an essential prerequisite to understanding the chemical reaction process and the eventual control/optimization of the energy conversion process. The PI has a record of accomplishment in the field of study and in combining research and teaching.

**TITLE:** Uncertainty Quantification in Large-Scale Ice Sheet Modeling and Simulation

**PRINCIPAL INVESTIGATOR:** Omar Ghattas, University of Texas
**CO-INVESTIGATORS:** Carsten Burstedde, University of Texas
Georg Stadler, University of Texas

**ABSTRACT:**
We request an in support of our research on quantifying uncertainties in large-scale inverse ice sheet models governed by creeping, viscous, incompressible flow models with strain rate- and temperature-dependent viscosity. The overall goal of our research program is to improve the understanding of the dynamics of polar ice sheet flows through solution of inverse problems to infer uncertain ice sheet model parameters from observed ice flow data, employing advanced high resolution forward simulations. The knowledge we will gain through our computations will improve the confidence in estimations of future changes to the dynamics and mass balance of polar ice sheets, and thus the accuracy of predictions of future sea level in climate change projections.

We employ a parallel state-of-the-art 3D full-Stokes forward ice flow model with Glen's law rheology, incorporating scalable multilevel preconditioned Newton-Krylov methods, high order mass-conserving finite element discretizations, and forest-of-octree adaptive mesh refinement. First and second-order sensitivities of ice flow observables with respect to unknown model parameter fields, such as the ice viscosity and the bedrock slipperiness, are determined through solution of adjoint ice flow models. The Bayesian inference framework is employed to describe the uncertainty in (discretized) ice flow parameter fields, including the basal slipperiness Coefficient and the Glen's law exponent, given uncertain surface velocities and prior densities on model parameters. The parameter uncertainty is represented by the posterior probability Density of the rheology and basal slipperiness parameters. Under the Gaussian assumption, the mean of this density is estimated by solving a regularized nonlinear least squares minimization problem to yield the maximum a posteriori point of the posterior pdf. A Hessian-free inexact Newton-conjugate gradient method is employed to solve the minimization problem, in which Hessian-vector products are computed by solving linearized forward and adjoint Stokes problem. Parameter covariance matrices are estimated by inverse Hessians, in conjunction with low rank approximations of the data misfit functional and Sherman-Morrison inverse formulas.

**TITLE:** Electrocatalyst Durability from First Principles Calculations

**PRINCIPAL INVESTIGATOR:** Jeffrey Greeley, Argonne National Laboratory (ANL)
**CO-INVESTIGATORS:** Subramanian Sankaranarayanan, ANL
Stephen Gray, ANL

**ABSTRACT:**
The proposed research will leverage new, highly parallelizable electronic structure (Density Functional Theory - DFT) codes and the computational resources available through the ALCC program to determine critical aspects of the stability and durability of electrocatalytic particles in the "non-scalable nano regime." Such properties have not previously been studied in detail because, by their very nature, the properties of nanosized structures in this size range cannot be extrapolated from the corresponding properties of either molecules (or, equivalently, small clusters) or bulk matter. It is relatively straightforward to probe either of these size extremes with standard DFT calculations, but intermediate regimes – with metallic or oxidized particles in the size range of ~2-4 nm – can only be described by explicit DFT calculations on massively parallel leadership-class computing resources. Our study will thus be one of the first examples of the use of rigorous electronic structure calculations to determine the properties of metallic and partially oxidized particles across the size range at which such properties cannot be extrapolated from the bulk. We note that this study is distinct from the active INCITE proposal of the PI. The INCITE work, while also concerned with metallic nanoparticles, is exclusively focused on their catalytic properties for carbon monoxide oxidation and does not address their stability in electrochemical environments, which is the focus of the present work.

In addition to providing important fundamental insight into the nanoscale size-dependent properties of electrocatalyst nanoparticles, the proposed work will also address critical questions concerning the durability and degradation of nano-sized fuel cell electrocatalysts. Catalytic fuel cell electrodes, generally composed of platinum or platinum alloy nanoparticles, are often very efficient in the chemical reactions that they carry out. However, they also suffer from significant performance losses due to long-term instabilities, platinum loss, and degradation in harsh electrochemical environments.

In spite of the critical technological importance of these degradative processes, though, many fundamental atomic-scale mechanisms of how the degradation occurs are not understood. In the proposed work, we will analyze such mechanisms for the competition between electrochemical metal dissolution and surface passivation via oxide formation.

The competition between these effects is key to understanding nanoparticle durability in electrochemical environments and is likely to be strongly particle size dependent; indeed, the effects are thought to change significantly in the critical size range of 3-4nm –precisely the non-scalable range that our calculations are capable of rigorously treating.

The calculations will be performed on Argonne's Blue Gene/P system using GPAW, a grid-based projector augmented wave DFT code from Jens Nørskov's group. *GPAW currently scales to 20% of Intrepid, 8-racks ~ 32,000 computational cores, and is reliably able to calculate energetics for metal and oxide nanoparticles with up to 15,000 valence electrons.* GPAW is presently used in a number of INCITE

and ALCC allocation at the Argonne Leadership Computing Facility (ALCF). Additionally, GPAW is the primary application in a Blue Gene/Q Early Science Program allocation.

As a secondary goal of our study, we will also perform classical molecular dynamics (CMD) simulations to treat oxidation and dissolution of platinum nanoparticles with diameters of tens of nanometers (millions of atoms). This "large-particle limit" will provide an important boundary condition for our DFT analyses of smaller particles.

**TITLE:** Controlling Nanoparticle Interactions to Engineer New Materials

**PRINCIPAL INVESTIGATOR:** Gary S. Grest, Sandia National Laboratories (SNL)
**CO-INVESTIGATORS:** Sanat K. Kumar, Columbia University
Dvora Perahia, Clemson University
Steve Plimpton, SNL
Mark O. Robbins, Johns Hopkins University
Mark Stevens, SNL

**ABSTRACT:**
The pathways to control assembly and integration of nanoparticles into new devices will be probed using multi-million atom molecular dynamics simulations. Nanoparticles encoded with organic ligands that allow control of the strength, length scale and directionality of the interparticle interactions will be investigated. Recent advances in synthesis have resulted in an unprecedented range of control of size and shape of nanoparticles. However, in order to take full advantage of these novel structures to build new architectures it is imperative to define the factors that control the interactions between the nanoparticles.

Large-scale molecular dynamic simulations will be used to probe the complex structure of nanoparticles assemblies, since it can systematically isolate specific factors that cannot be resolved experimentally. With access to petascale computational resources, we will for the first time be able to capture the essential time and length scales that dominate the physics of nanoparticle assembly and integration into polymer matrices. These simulations will allow us to zoom into the interaction regions, providing the needed molecular level understanding. The present study will combine fully atomistic and coarse grained simulations to correlate the interactions between nanoparticles and between nanoparticles and their surroundings with the properties of nanoparticles assemblies. Starting with atomistic simulations and moving up in length and time scale using coarse grained models; the team will probe nanoparticle assemblies from individual particles with their specific chemical modifications up to the macroscopic scale, where the nanoparticles are assembled into devices. This work will address the two major barriers to integrating nanoparticles into a range of advances devices, controllably dispersing and organizing them within durable matrices while retaining their unique properties.

**TITLE:** First principles-based design of novel solar thermal fuels

**PRINCIPAL INVESTIGATOR:** Jeff C. Grossman, MIT

**ABSTRACT:**
Solar thermal fuels, which store energy from the sun in the chemical bonds of molecules, are a tantalizing energy storage prospect: in principle they are 100% renewable, produce no emissions, are easily transportable in the form of liquids or powders, and can be recharged without any special equipment. However, adaptation of solar fuels as a viable, low-cost, large-scale means of energy storage will require the discovery of new materials other than the one known case based on Ru that can perform the process over many cycles with no degradation. Here we propose a novel approach to the discovery and design of solar thermal fuels using a first principles-based high-throughput screening method to search several thousand known photochromic molecules for promising candidates. In addition to efficiently screening known molecules, the proposed technique will lead to a deeper understanding of the molecular and electronic properties that give rise to the desired photoactive behavior, thereby enabling intelligent design of completely new molecules and molecular systems for solar energy storage applications.

**TITLE:** High Resolution Design-Cycle CFD Analysis, Supporting CO2 Compression Technology Development

**PRINCIPAL INVESTIGATOR:** A.D. Grosvenor, Ramgen Power Systems, LLC

**ABSTRACT:**
The use of fossil fuels worldwide requires developing economically viable technology to sequester CO2 as one means of curbing global warming. International commitments require "research on, and promotion, development and increased use of … carbon dioxide sequestration technologies..." One major expense in sequestering CO2 is compressing it to high pressures. Addressing this, Department of Energy goals include developing "novel concepts for the compression of large volumes of CO2."

Ramgen Power Systems shock compression technology employs supersonic aerodynamic design techniques projected to dramatically decrease the size, cost and power required for compressing CO2. This promising breakthrough in turbomachinery efficiency and cost is achieved by combining aerodynamics and mechanical engineering in new ways. To optimize the technology, very high grid resolution is required to capture the 3D shock distributions and accurately model the resulting compressible viscous flow behavior.

After reviewing papers on the technology including early rotating rig tests validating Computational Fluid Dynamics (CFD) predictions, DOE Secretary Steven Chu identified the use of supercomputers as a means to shorten the time required to optimize the design and to reach product performance targets.

Ramgen works closely with the Oak Ridge Leadership Computing Facility (OLCF), the DOE Office of Fossil Fuels and Office of Science, and NETL to move the technology along its development curve at a fast pace.

In addition to lowering the costs of CCS with the CO2 compressor, advancing the Ramgen shock wave based technology also promises a major breakthrough in small engine performance and cost. The engine holds significant promise for reducing greenhouse gases as support for renewable technologies and by using dilute waste methane as fuel at industrial sites.

**TITLE:** High Resolution Design-Cycle CFD Analysis, Supporting CO2 Compression Technology Development

**PRINCIPAL INVESTIGATOR:** Allan D. Grosvenor, Ramgen Power Systems, LLC

**ABSTRACT:**
We were directed to the Oak Ridge Leadership Computing Facility (OLCF) by Secretary Chu, the Assistant Secretary for Fossil Energy and the Office of Science, and we have spent a year running computations, and scalability studies, on OLCF systems including Smoky and Jaguar (XT4 and XT5), as well as Lens for post-processing/visualization. This computational modeling work has accelerated our development efforts and has shown the tremendous value of the capability in place at ORNL. The completion of this work is critically important to the development of the Ramgen technology on the timeframe required to achieve DOE climate change goals.

Shortly after Dr. Steven Chu was confirmed as the Secretary of Energy, he reviewed technical papers on the Ramgen technology. The Secretary subsequently identified the technology as being highly important for meeting DOE goals to reduce the cost of Carbon Capture and Sequestration (CCS) and he identified the use of supercomputers as a means to shorten the time required to optimize the design and to reach product performance targets.

This proposal is a continuation of that transformational work and the breakthrough progress we are making. If Ramgen is unable to complete the computational work initiated at ORNL, it will be a major setback for this DOE-supported project.

**TITLE:** Simulating Regional Climate at Convection Permitting Resolution

**PRINCIPAL INVESTIGATOR:** Greg Holland
**CO-INVESTIGATORS:** Cindy Bruyère, National Center for Atmospheric Research
James Done, National Center for Atmospheric Research

**ABSTRACT:**
This project will demonstrate the opportunities and challenges of simulating regional climate at sufficient resolution to resolve individual thunderstorm circulations. Significant simulation benefits are anticipated at this convection-permitting resolution. Of particular interest is the impact on the regional climate through improved treatment of the upscale impact of convective weather systems.

Foci for the simulation will be the water-snowpack assessments for the mid and western US, wind energy assessments, and high-impact weather such as winter storms and hurricanes. The experience gained at a resolution that is set to be the standard for the next generation of regional climate models represents an essential step towards our overarching goal to better quantify the frequency, duration, and intensity of extreme events under climate variability and change.

The major focus on simulation of the 2005 hurricane season provides a thorough test of convection-permitting resolution on climate timescales due to the huge sensitivities of hurricane formation, structure, intensification, maximum intensity, and dissipation to environmental conditions. Further, hurricane upscale impacts on the large-scale environment are one of the major current issues with future climate predications at decadal scales.

This ambitious project provides for the first time high-resolution regional climate information over a sufficiently long period to assess seasonal statistics, and provides a genuine test of the requirements for future supercomputing systems. In establishing the feasibility of high-resolution climate models with focus on weather extremes this work will advance our understanding of Earth's climate, for national emergencies, and broaden the community of researchers capable of using leadership computing resources.

**TITLE:** Petascale Quantum Monte Carlo Calculations of Strongly Correlated and Energy Storage Materials

**PRINCIPAL INVESTIGATOR:** Paul R. C. Kent, Oak Ridge National Laboratory
**CO-PRINCIPAL INVESTIGATORS:**
David M. Ceperley, University of Illinois
Jeongnim Kim University of Illinois
Lubos Mitas, North Carolina State University
Henry Krakauer College of William and Mary
Shiwei Zhang College of William and Mary

**Abstract:**
We propose quantum Monte Carlo (QMC) calculations on classes of materials of direct interest to the DOE, strongly correlated systems and energy storage and conversion materials. Over the last two decades, QMC research has had a significant impact on condensed matter physics, materials science, chemical physics and nanoscience, beginning with the 1980 calculation of the correlation energy of the electron gas on the Cray computers. In the past decade, QMC has played an important role in benchmarking other methods for calculating the properties of systems of correlated electrons in real materials, for example, materials at high pressure. Now, with increases in computer capability and much improved algorithms, QMC can address many difficult problems directly from first principles.

The materials we propose to study focus on strongly correlated systems including transition metal oxides, and possible materials for energy storage. They represent some of the most challenging problems in quantum physics, chemical physics, materials research and condensed matter physics. Driven by the physics of interacting electrons, they do not fit any set of traditional paradigms or mean-field models. Although mainstream approaches such as density functional theory (DFT) can provide a good starting point to understand these phenomena, current approximations are often greatly limited in accuracy, even when empirical corrections from experiment are applied. QMC methods are uniquely applicable to solid-state materials, through nanostructures, to the molecular state: systematically robust and predictive calculations are not yet within reach by other more traditional electronic structure calculations. QMC methods, although less mature than the more developed DFT and quantum chemistry approaches, represent a promising new general approach to correlated materials problems. Our proposed calculations are for systems that are representative of broad classes of correlated materials problems and we aim to make strong contact with experiment. Thus, the projects we propose here have a large component of high-risk, high-payoff simulation.

The proposal team has been a very active user of the DOE leadership computing facilities. Starting from DOE funding in 2008 under the Endstation program, we have continuously developed the software to effectively and efficiently utilize the petaflop platforms. QMC methods have strong capacity for excellent parallel scaling. However, because of branching in the random walks and the complex nature of random walkers (or the so-called trial wave functions), effective parallelization at the petascale and beyond in fact presents significant challenges, i.e. parallelization is non-trivial. With a major sustained development effort, computational efficiency and ability to scale to larger fractions of the resources have steadily improved.

**TITLE:** Large-eddy simulation for turbomachinery – advancing the state-of-the art

**PRINCIPAL INVESTIGATOR:** Gorazd Medic, United Technologies Research Center
**CO-INVESTIGATORS:** Pratt & Whitney

**Abstract:** This project will explore the application of large-eddy simulation to realistic three-dimensional turbomachinery configurations. Case studies will focus on the centrifugal compressor and low-pressure-ratio axial fan, with the additional geometries of interest being high- and low-pressure turbine. Centrifugal compressors are a key technology in many of UTC products: commercial chillers (Carrier), aircraft environmental control systems, aircraft auxiliary power units, and fuel pumps (Hamilton Sundstrand, Pratt & Whitney Rocketdyne), and in rotorcraft and business jet engines (Pratt & Whitney Canada). An efficient low-pressure-ratio axial fan is a key component for the geared turbofan architecture that Pratt & Whitney has developed for its next generation of commercial jet engines to enable lower fuel burn than traditional designs.

Large-eddy simulation is particularly attractive for modeling turbulent flows in turbomachinery because these flows contain several features that have over the years proven to be a challenge for RANS turbulence models widely used in industry. These features include: strong rotational effects due to the high rotational speeds; strong curvature of the hub and shroud surfaces yielding highly 3-D flows in the endwall regions; large tip-clearance vortices that typically migrate downwards and occupy a significant portion of the flow passage; and the presence of flow separation, especially at off-design conditions. For flows that encounter transition from laminar to turbulent flow, such as is in the case of the low-pressure ratio fan, modeling is entirely based on tedious calibration with experiments for various modes of transition further reducing the predictive capability of RANS framework. Our ability to better understand the flow physics in these specific product components using wall-resolved large-eddy simulation on grids of sufficient resolution will help lead future design improvements and will be critical to improved energy efficiency of our products going forward.

**TITLE:** Prediction of Supersonic Jet Noise Using Large Eddy Simulation

**PRINCIPAL INVESTIGATOR:** Parviz Moin, Stanford University

**ABSTRACT:**
This project aims to perform high fidelity, Large-Eddy Simulations (LES) of supersonic jet noise from complex geometry nozzles. One of the major problems confronting the aircraft industry is the aerodynamic noise generated by engine exhaust jets and airframes, particularly during take-off and landing. The noise problem has been a major issue for high-speed commercial aircraft (e.g., the Concorde) and for military aircraft, both for impact on communities surrounding airports and military bases, and on the crew stationed on aircraft carrier decks.

Even the most advanced hearing protection devices cannot offer adequate protection from 150 dB noise produced by present-day high-performance aircraft motivating the need to reduce acoustic emissions at their source. For high-speed turbulent jets, both large-scale coherent structures and fine-scale turbulent mixing contribute to the overall exhaust noise. In addition, shock-associated noise is an important component of supersonic jet noise making jet noise prediction a complex, multiscale problem. LES adapted to extreme scale computing resources offers a unique opportunity for new insight into this difficult scientific problem, by simultaneously predicting both the far-field noise as well as details of the noise generating turbulent eddies with a fidelity beyond what is possible in laboratory experiments.

To reduce jet noise at its source, various schemes have been proposed to alter the jet flow by making modifications to the jet nozzle, including the addition of tabs, chevrons, and even micro-jets, situated azimuthally around its lip. Chevroned nozzles are known to reduce the overall sound pressure level of the jet flow, but shift the noise to higher frequencies, although the physical reasons for this are not yet fully well understood. Shaped and beveled nozzles have also been candidates for noise reduction, but more importantly, may play a role in changing the directivity of the emitted sound. Some combinations of the above techniques may reduce the sound levels without impacting fuel economy and performance, or at least result in an acoustic signature tailored to a particular application. Even though the small scales generated in the initial jet shear layers by these nozzle modifications do not contain much energy, they do dramatically influence the development of the large coherent motions downstream and thus alter the production of far-field noise. As a result, the precise three-dimensional details of the nozzle geometry must be carefully resolved.

While aeroacoustic calculations traditionally have relied upon structured meshes yielding low numerical dissipation, the current investigations uses the unstructured finite volume LES solver "CharLES" in order to resolve the complex geometry. The CharLES solver, however, minimizes dissipation through the use of novel widened numerical stencils based on higher-order polynomial expansions, in some cases recovering dissipation levels typical of structured meshes. This approach, coupled with methods to project acoustics to the far-field (e.g., via a Ffowcs Williams-Hawkings (FWH) surface), has already demonstrated significant and efficient predictive capability for simple round and shaped nozzles, but with the computational resources afforded by the Argonne Leadership Computing Facility (ALCF) is now extended to increasingly complex and realistic three-dimensional geometries. Four simulations of a heated/unheated supersonic turbulent jet issuing from a 2:1 aspect-ratio rectangular nozzle with and

without chevrons are planned with the aim of investigating the effects of the chevrons and heating on the noise produced in supersonic turbulent flow from a rectangular nozzle. The simulated nozzle geometries precisely match those under experimental investigation at the NASA Glenn Research Center so that the far-field simulation results can be validated against laboratory measurements. Resolved simulations of chevrons are expected to reveal new insight into how the enhanced shear layer mixing due to chevrons sustains itself and, in turn, prioritize possible noise-mitigation strategies critical to the design and viability of next-generation supersonic transport vehicles.

**TITLE:** Non-icing Surfaces for Cold Climate Wind Turbines

**PRINCIPAL INVESTIGATOR:** Masako Yamada, General Electric

**ABSTRACT:**
Prevention of ice accretion and adhesion on surfaces is relevant to many applications, including wind turbine blades, aircrafts, oil and gas rigs, heat exchangers, transmission lines, buildings and boats. In many cases in addition to improving operation safety and reducing cost, reduction of ice buildup can lead to increased energy efficiency. For instance, ice buildup on wind turbine blades in cold climates (T< -20C) drastically reduces the efficiency of power generation, often requiring turbine shutdown. Furthermore, even a small layer of ice on the wind turbine sensors, such as anemometers, can lead to an underestimation of the wind speed by 30% causing additional energy losses. It should be noted that there is tremendous potential to implement wind power in cold climates in Northern and Central Europe, Northern America and Asia. However, the potential to generate wind power in cold climates has not been fully realized due to the lack of adequate ice mitigation strategies. Many of the current approaches, such as the heat-based methodologies commonly used for cold climate wind turbine blades, are based on *active* de-icing or anti-icing processes requiring additional energy to generate heat. Therefore, development of *passive* ice mitigation strategies such as ice resistant coatings, which do not require additional energy consumption, is highly desirable.

General Electric through its Global Research facilities has actively sponsored a multi-year internal activity to enable innovative passive coating based solutions to mitigate icing problems in a variety of applications, including wind turbines. The goal of the proposed simulations is to explain, and ideally guide, the core experimental work. Limited simulations comprising about 1000 molecules (total dimension of only a few nanometers) have been conducted in-house, in collaboration with the experimental team, but available resources have not been sufficient to probe the size and time scales that are relevant to their interests.

GE Global Research proposes using molecular dynamics (MD) on the Jaguar Cray XT5 at Oak Ridge National Lab to gain understanding of icephobicity on a molecular level. The objective of the proposed activity is to probe the early stages of ice formation on three particular surfaces with varying degrees of hydrophobicity, specifically to understand how certain surfaces hinder the formation of ice.

Hydrophobicity is a well-studied field, and many such surfaces have been synthesized for room temperature use, including superhydrophobic surfaces that have very high water contact angles (reduction of water/surface interaction area) leading to water droplets beading up and rolling off. Extending the superhydrophobic behavior of these coatings to sub-freezing temperatures has been a matter of significant debate over the last few years. Surfaces that are —superhydrophobic at room temperature may not be icephobic at freezing temperatures. In contrast, a —hydrophilic surface at room temperature may prove —icephobic under certain conditions. This complexity is borne of the multiple physical mechanisms that govern ice inhibition, including: 1) delay in freezing time until a critical ice nucleus forms, 2) depression of freezing temperature and 3) reduction of water/surface adhesion strength for improved shedding.

Predicting icephobicity is not a simple matter of calculating static water/surface free-energy. First, that calculation is not easy given that surface effects can penetrate deeper than the nominal interaction distance and must account for conformational changes of several layers of water. Moreover, freezing is a kinetic process, and the drivers for ice formation depend on additional factors such as absolute temperature, cooling rate, droplet volume and droplet shape.

The use of the world-class Jaguar Cray XT5 can push the limits of MD to make the proposed simulations possible, but it is still a formidable computational challenge, as the proposed system spans orders of magnitude in physical dimension (> 10^3 orders) and time (> 10^8 orders).

**TITLE:** Sensitivity and uncertainty of precipitation of a climate model

**PRINCIPAL INVESTIGATOR:** Laura Zamboni, Argonne National Laboratory

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**Abstract:**
Physical processes occurring at spatial and temporal scales not resolved by Atmospheric General Circulation Models (AGCMs) are a major source of uncertainty (sensitive dependence) in explorations of natural climate variability, seasonal predictions, and climate change assessments, since the values of the corresponding AGCMs' parameters are not uniquely defined.

The primary aim of the proposed research is to quantify the magnitude of this uncertainty for the seasonal precipitation and its variability in the present climate. The analysis will be conducted with the High Resolution Atmospheric Model (HIRAM) developed at the Geophysical Fluid Dynamics Laboratory (GFDL) for the entire globe at a 100 km horizontal resolution. This is remarkably high for this type of study.

We propose to perform ensembles of simulations by systematically perturbing certain parameters in HIRAM. These include the entrainment rate in convective clouds, the ice - fall - speed, the threshold for the occurrence of precipitation in both convective and stratiform clouds, and the critical droplet radius in stratiform clouds.

We will assess whether sensitive dependence and internal variability can be separated at the regional scale, and we will establish the functional form of the sensitivity to individual parameters.

The proposed research contains several innovative aspects: the focus on precipitation and its variability, the high horizontal resolution, and the outstanding quality of the atmospheric model used. This research will be of great value to the research community and provide an uncertainty estimate to be considered for risk assessment and water management worldwide