

Title: Multiphase Flow Simulations of Nuclear Reactor Flows

Principal Investigator: Igor Bolotnov (North Carolina State University)

Co-investigators: Jun Fang (Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)

Allocation: 130,000,000 core-hours on Mira

Research Summary:

Direct numerical simulation (DNS) of turbulent two-phase flows at a leadership computing facility allows achievement of unprecedented level of detail and can answer fundamental questions about the interaction between the complex and evolving interfaces between flow phases and turbulence. The detailed simulation of all turbulent structures using a DNS approach as well as interface evolution in turbulent flows (in the form of bubbles, droplets, and wavy interfaces between liquid and steam in various flow regimes) will allow the collection of statistical information about two-phase flow parameters at unprecedented Reynolds numbers and levels of detail. An advanced data collection approach coupled with interface-tracking methods will help process large data sets provided by the simulations. Three subprojects will generate two-phase flow results highly relevant to nuclear reactor flows, including (i) bubbly flow through pressurized water nuclear reactor fuel bundles with complex geometry spacers, (ii) complex two-phase flow regimes (slug and churn flow) as well as (iii) droplet interactions with reactor structures during accident scenarios. Major statistical parameters, such as flow rate, mean velocity and gas volume fraction will be assessed against experimental data while the higher order statistics will bring new knowledge about two-phase flows. With the help of the Leadership Computing Facilities detailed data will be provided for new closure laws which will allow reliable application of multiphase computational fluid dynamics to nuclear reactor systems. This will improve the safety margin predictions for existing light water reactors and facilitate the development and design of next generation energy systems.

Title: Analysis and Mitigation of Dynamic Stall in Energy Machines

Principal Investigator: Anupam Sharma (Iowa State University)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)

Allocation: 51,500,000 core-hours on Mira

Research Summary:

Large unsteady loads caused due to dynamic stall in rotating blades of power generation turbomachines can lead to fatigue or catastrophic failure, reduced aerodynamic performance, and increased acoustic emissions. In particular, this project focuses on wind turbines that operate in the highly turbulent atmospheric boundary layer (ABL) with large spatial and temporal gradients. Blade failures due to dynamic stall are curtailing the growth of wind energy, which is currently the primary renewable energy source in the US and in the world. While the general characteristics of dynamic stall have been known for decades, the flow phenomena that occur during stall incipience, and which ultimately lead to stall, are not well understood. The complex, unsteady boundary layer behavior at stall onset holds the key to understanding and subsequently mitigating, dynamic stall; to date it has not been investigated in careful detail due primarily to lack of resources. This project proposes to use wall-resolved large eddy simulations to improve our fundamental understanding of the fluid dynamic processes that occur in the boundary layer near stall incipience, and also investigate novel ideas to passively mitigate dynamic stall for wind turbine and gas turbine applications. Several innovative mechanisms, including wavy leading edge, vortex generators, pressure-side tabs (Gurney flaps), and back-flow flaps will be evaluated for their ability to mitigate dynamic stall.

Title: High-Throughput Calculation of Materials Properties at Finite Temperature toward Predicting Novel Thermoelectrics

Principal Investigator: Chris Wolverton (Northwestern University)

Co-investigator: Yi Xia (Argonne National Laboratory)

ALCC allocation:

Site: National Energy Research Scientific Computing Center (NERSC)

Allocation: 54,000,000 core-hours on Cori

Research Summary:

Over the past decade, as part of the Materials Genome Initiative, several high-throughput computational databases of materials properties have been developed, using first-principles calculations of hundreds of thousands of compounds. These databases have been used to discover new materials for a wide variety of applications, e.g., metallic alloys, Li-ion battery electrodes and electrode coatings, thermoelectrics, superconductors, and photovoltaics. While evidently useful, currently available databases are limited to materials properties calculated at idealized conditions of zero temperature. Most finite-temperature properties such as heat capacity, thermal expansion coefficients, thermal conductivities, etc. are yet to be computed on a large scale; the primary reason being lattice dynamics simulations needed to model vibrations of atoms in a crystal are extremely computationally expensive. However, recently developed methods, namely the compressive sensing lattice dynamics (CSLD) method, enables the accurate calculation of vibrational properties of a material at a fraction of the computational cost of conventional methods. This project proposes to use CSLD within the framework of the Open Quantum Materials Database (OQMD) to calculate finite-temperature properties in a high-throughput fashion for thousands of compounds. In particular, the project will screen for compounds with low thermal conductivity in an effort to discover new efficient thermoelectric materials. Additionally, all resulting output from this project will be made freely available through the OQMD for the benefit of the wider scientific community.

Title: Semileptonic B- and D-meson form factors with high precision

Principal Investigator: Ruth Van de Water (Fermi National Accelerator Laboratory)

Co-investigators:

John Laiho (Syracuse University)
Doug Toussaint (University of Arizona)
Aida El Khadra (University of Illinois)
Andreas Kronfeld (Fermi National Accelerator Laboratory)
Steven Gottlieb (Indiana University)
Carleton DeTar (University of Utah)
Elvira Gamiz (University of Granada)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 177,000,000 core-hours on Mira and 70,000,000 core-hours on Theta

Research Summary:

Precise calculations of hadron properties are necessary to make progress in elementary particle physics. Although the Standard Model of particle physics has been enormously successful in describing the sub-atomic world, several mysteries connected to quark interactions, neutrino physics, and cosmology cannot be reconciled without additional particles and/or new forces among the known particles. One longstanding mystery is the preponderance of matter over antimatter in the present universe. To explain the matter-dominated universe, interaction rates must differ for matter and antimatter. (In particle physics, this circumstance is known as charge conjugation parity symmetry violation or “CP violation”.) The Standard Model has CP-violating processes, but they are not strong enough to explain today's universe. Therefore, further CP-violating interactions must exist. According to many hypotheses aimed at solving these mysteries, new sources of CP violation arise from quark interactions. This idea has motivated a decades-long search for evidence of such interactions in numerous experiments worldwide. The experiments do not, however, detect quarks, which are always bound into larger particles called hadrons. The connection between quarks and hadrons must be computed numerically with lattice quantum chromodynamics (QCD). This project team has a long record of performing world-leading lattice-QCD calculations in the realm of CP violation. This project builds on previous work to achieve greater precision than ever before. Several indications of new CP-violating interactions exist in the data. New experiments to study them with greater scrutiny are underway and starting soon: without the proposed work, these experiments will not be able to discern whether such indications are real.

Title: Modeling Fusion Plasma Facing Components

Principal Investigator: Brian Wirth (Oak Ridge National Laboratory/University of Tennessee)

Co-investigators: David Bernholdt (Oak Ridge National Laboratory)
Blas Uberuaga (Los Alamos National Laboratory)
Rick Kurtz (Pacific Northwest National Laboratory)
Aidan Thompson (Sandia National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 80,000,000 core-hours on Theta
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 60,000,000 core-hours on Titan
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 25,000,000 core-hours on Cori

Research Summary:

The realization of fusion as a practical, 21st Century energy source requires improved knowledge of plasma surface interactions and the materials engineering design of component systems to survive the incredibly extreme heat and particle flux exposure conditions of a fusion power plant. The objective of this proposal is to further advance understanding of the response of tungsten, the proposed material for the ITER diverter, to low energy mixed H-He plasma exposure.

Title: Increasing the Scale of Implicit Finite Element Analyses

Principal Investigator: Todd Simons (Rolls-Royce Corporation)

Co-investigators: Seid Koric (University of Illinois at Urbana Champaign)
Robert Lucas (Livermore Software Technology Corporation)
Ting-Ting Zhu (Cray Incorporated)

ALCC allocation:
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 10,000,000 core-hours on Titan

Research Summary:

Increasing the scale of Finite Element Analysis (FEA) is critical for the research and development needed to enable virtual prototyping of ever larger and more complicated systems, including the gas turbine engines manufactured by Rolls-Royce. This will reduce design cost and accelerate the deployment of such systems, enabling the United States to maintain its economic and intellectual leadership. This proposal builds on an ongoing collaborative effort Rolls-Royce is leading with the University of Illinois, Cray Inc., and Livermore Software Technology Corporation. This project endeavors to increase both the scale and sophistication of FEA models, and the resources that can be brought to bear on them. Towards that end, Rolls-Royce has developed a family of finite element models of a gas turbine engine with generic geometry, and representative boundary conditions and model size. The conditional stability requirement in an explicit formulation of this model would require weeks of run time. Therefore, this project is investigating LS-DYNA's implicit solver on leadership class computing resources, attempting to reduce the time-to-solution to a matter of hours. Access to leadership class computing resources will enable researchers to study behavior of the generic engine model and FEA software at a scale beyond that otherwise accessible, and then address the challenges encountered. The project team has had early success with smaller models using NSCA's Blue Waters, but are constrained by the limited memory per computing node. Success in this effort will be a major step towards virtual certification of engines and enhancing both the efficiency and safety of aviation.

Title: Study of a Disrupting Plasma in ITER

Principal Investigator: Stephen Jardin (Princeton Plasma Physics Laboratory)

Co-investigators:
Nathaniel Ferraro (Princeton Plasma Physics Laboratory)
Isabel Krebs (Princeton Plasma Physics Laboratory)
Jin Chen (Princeton Plasma Physics Laboratory)

ALCC allocation:
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 40,000,000 core-hours on Cori

Research Summary:

The ITER fusion experiment under construction in Cadarache, France will heat plasma to temperatures exceeding those on the sun at sufficient pressure for fusion reactions to occur. The high-temperature, high-pressure plasma is isolated from tokamak chamber walls by strong magnetic fields produced primarily by some of the world's largest electromagnets. Large electrical currents flowing in the tokamak plasma itself produce additional magnetic fields that are essential. The Princeton Plasma Physics Laboratory has developed a class of modeling codes, called magneto-hydrodynamic (MHD) codes, which operate on some of the world's most powerful computers. These MHD codes can predict many aspects of the behavior of the plasma within a tokamak, and in particular can identify conditions in which instability can develop that would disrupt the normal operation. This proposal is to apply these codes to the present ITER design to confirm expected regions of stable operation.

Title: The Real World of Real Glue

Principal Investigator: Robert Edwards (Jefferson Lab)

Co-investigators:

Raul Briceno (Old Dominion University)
Jozef Dudek (College of William and Mary)
Balint Joo (Jefferson Lab)
Michael Peardon (Trinity College, Dublin)
Sinead Ryan (Trinity College, Dublin)
Christopher Thomas (DAMTP, Cambridge University)
David Wilson (Trinity College, Dublin)
Frank Winter (Jefferson Lab)

ALCC allocation:

Site: Oak Ridge Leadership Computing Facility (OLCF)

Allocation: 96,000,000 core-hours on Titan

Research Summary:

Quantum Chromodynamics (QCD), the theory of the strong nuclear force, predicts that the majority of the mass observed in the visible universe comes not from the quarks that build matter, like protons and neutrons, but instead from the “glue” that binds the quarks. However, this “glue” has not been directly observed. There are world-wide efforts to determine the spectrum of quarks that form sub-atomic particles, and exploring the spectrum of QCD is a flagship project of the Thomas Jefferson National Accelerator Facility (Jefferson Lab). Studies of the excited meson spectrum is of particular interest because it may reveal the presence of “exotic” mesons, which would be a tell-tale signal of the glue. The new GlueX experiment at Jefferson Lab, which commenced operations in 2017, has been built to discover and explore properties of exotic meson states. This computational research project aims to compute the excited-state meson spectrum, and specifically predict from theory and simulation the masses of possible exotic meson states in advance of experimental results from GlueX. These calculations will guide future GlueX experimental runs and advance our understanding of matter and fundamental physics.

Title: Investigating Climate-biogeochemistry Feedbacks with the Energy Exascale Earth System Model (E3SM v1)

Principal Investigator: Peter Thornton (Oak Ridge National Laboratory)

Co-investigators: David Bader (Lawrence Livermore National Laboratory)
Ruby Leung (Pacific Northwest National Laboratory)
Katherine Calvin (Pacific Northwest National Laboratory)
William Riley (Lawrence Berkeley National Laboratory)
Matthew Maltrud (Los Alamos National Laboratory)
Mark Taylor (Sandia National Laboratory)

ALCC allocation:

Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 70,000,000 core-hours on Cori and 80,000,000 core-hours on Edison

Research Summary:

The project uses a state-of-the-art coupled earth systems model to explore interactions of the land and ocean components of the biosphere with Earth's physical climate system. Connections between water, energy, and carbon cycles are considered, as are the biological dependencies of those interactions on nutrients, such as nitrogen and phosphorus. The knowledge gained from this project will improve predictions of the evolution of the global climate.

Title: Scaling LHC proton-proton collision simulations in the ATLAS detector

Principal Investigator: Eric Lancon (Brookhaven National Laboratory)

Co-investigators: Taylor Childers (Argonne National Laboratory)
Paolo Calafiura (Lawrence Berkeley National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 80,000,000 core-hours on Theta
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 80,000,000 core-hours on Titan

Research Summary:

The Standard Model of particle physics is being tested with ever increasing precision in proton-proton collisions by the ATLAS experiment at the Large Hadron Collider (LHC). While the masterpiece of the model, the Higgs boson, has been discovered at the LHC, many fundamental questions have no answer within the present understanding of particle physics: Why is there more matter than antimatter; what is dark energy; why do neutrinos have mass? To answer these questions, precision measurements performed at the LHC need to be compared with precision model simulations, which are computationally demanding. DOE's leadership class supercomputers are becoming a necessity to ensure the U.S. physics program at the LHC meets its scientific goals. The computing and data challenges will increase at least by an order of magnitude with the High-Luminosity LHC looming on the horizon. This project will drive new software optimization efforts to improve the computational efficiency of precision model simulations and will provide researchers with 160 million simulated collisions.

Title: Hadronic Light-by-light Scattering and Vacuum Polarization Contributions to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions

Principal Investigator: Thomas Blum (University of Connecticut)

Co-investigators:

Luchang Jin (University of Connecticut)
Norman Christ (Columbia University)
Taku Izubuchi (Brookhaven National Laboratory)
Christoph Lehner (Brookhaven National Laboratory)
Chulwoo Jung (Brookhaven National Laboratory)
Peter Boyle (University of Edinburgh)
Antonin Portelli (University of Edinburgh)
Masashi Hayakawa (University of Nagoya)
Andreas Juettner (University of Southampton)
Aaron Meyer (Brookhaven National Laboratory)
Mattia Bruno (Brookhaven National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 162,000,000 core-hours on Mira

Research Summary:

The muon is a heavy cousin of the electron. Its magnetic moment is an intrinsic property that has been measured experimentally and computed using the Standard Model to high accuracy. But the experimental measurement and the computed value disagree by three standard deviations, which could indicate that a new theory is needed to explain the discrepancy. This research project, along with new experiments at Fermilab in the U.S. and later at JPARC in Japan, will reduce uncertainties enough to settle the matter. The discovery of new physics would dramatically reshape our understanding of the universe.

Title: High-Fidelity Simulation for Molten Salt Reactors: Enabling Innovation through Petascale Computing

Principal Investigator: Elia Merzari (Argonne National Laboratory)

Co-investigators: Aleksandr Obabko (Argonne National Laboratory)
Paul Fischer (Argonne National Laboratory)
Lane Carasik (Kairospower.com)

ALCC allocation:
Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 140,000,000 core-hours on Mira

Research Summary:

Amid an increase in cost of traditional nuclear reactor designs, in recent years advanced reactor concepts based on molten salt coolants have emerged as an attractive solution capable of increasing inherent safety while reducing cost. An example is the fluoride-salt-cooled, high-temperature reactor (FHR) that can be deployed with robust safety, affordable cost, and flexible operation. While promising, molten salt technologies have historically received much less attention than competing designs (e.g., sodium reactors). Consequently, there is a far smaller amount of heuristic and modeling knowledge compared to other reactor designs. Further development of the FHR technology will involve design optimization of key systems, structures, and components for commercialization. The main challenge is to use appropriate tools measured by the code's fidelity to the governing physics involved at all levels of the design iteration and optimization process, from the lowest-length scale up to the full reactor plant scale. This proposal addresses this challenge, providing much-needed high-fidelity data to inform lower-fidelity models. The project will focus on critical components of the FHR reactor: the core and the heat exchangers. For both cases researchers will conduct high-fidelity simulations with Nek5000. These will generate invaluable datasets that will allow the exploration of a broader design space, ultimately fostering innovation.

Title: Large Scale Simulations of Heterogeneous Materials for Energy Conversion Applications

Principal Investigator: Giulia Galli (University of Chicago & Argonne National Laboratory)

Co-investigators: Francois Gygi (University of California, Davis)
Marco Govoni (Argonne National Laboratory)
Juan de Pablo (University of Chicago & Argonne National Laboratory)

ALCC allocation:
Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 100,000,000 core-hours on Mira

Research Summary:

The mission of the Midwest Integrated Center for Computational Materials (MICCoM), one of the computational materials science centers funded by DOE/BES, is to develop and disseminate open source software, validation procedures and data to predict and design functional materials for energy conversion processes. The Center's vision is built on the premise that the discovery and design of innovative materials requires the ability to predict transport and dynamical properties of complex systems across multiple length scales. The distinctive objectives of the center are to: (i) develop interoperable codes for simulation of materials at multiple length and time scales; (ii) focus on heterogeneous materials, inclusive of defects, interfaces and building blocks assembled out of equilibrium; (iii) focus on spectroscopic and transport properties. This project will undertake simulations to advance objectives (i) and (ii) for specific heterogeneous, semiconducting materials for solar and thermal energy conversion applications.

Title: Predictive Modeling and Machine Learning for Functional Nanoporous Materials

Principal Investigator: J. Ilja Siepmann (University of Minnesota)

Co-investigators:

Laura Gagliardi (University of Minnesota)
Jason Goodpaster (University of Minnesota)
Chris Knight (Argonne National Laboratory)
Christopher Mundy (Pacific Northwest National Laboratory)
Donald Truhlar (University of Minnesota)
Yongchul Chung (Pusan National University)

ALCC allocations:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 42,000,000 core-hours on Mira
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 16,000,000 core-hours on Cori

Research Summary:

Improving the understanding and selection of nanoporous materials for separation and catalytic processes in the chemical, biorenewable, and petrochemical industries has tremendous potential societal benefits. An interdisciplinary, collaborative team will use predictive hierarchical modeling and machine learning to accelerate the discovery and design of nanoporous materials for a variety of energy-related applications. Depending on the complexity of the interactions between the guest molecules and the host material, the team employs a variety of computational techniques that range from high-level quantum-mechanical calculations to simulations using periodic electronic density functional theory and parameterized force fields. The proposed research activities are aimed at extending force fields to larger classes of porous materials, at developing machine-learned models for the prediction of mixture adsorption behavior, at understanding the effects of solvent removal (activation) for metal-organic frameworks, and at developing quantum-mechanical embedding methods for accurate modeling of magnetic properties in metal organic frameworks with potential applications for air separation.

Title: The AMS Experiment: Monte Carlo Simulations for the Study of the Anti-Deuteron Flux in Cosmic Rays

Principal Investigator: Samuel Ting (Massachusetts Institute of Technology)

Co-investigators:

Baosong Shan (CERN)
Andrei Kunine (Massachusetts Institute of Technology)
Zhili Weng (Massachusetts Institute of Technology)
Vitali Choutko (Massachusetts Institute of Technology)

ALCC allocation:

Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 100,000,000 core-hours on Cori

Research Summary:

The Alpha Magnetic Spectrometer (AMS-02) is a state-of-the-art particle physics detector that has operated as an external module on the International Space Station since 2011. It uses the unique environment of space to study the universe and its origin by searching for antimatter and dark matter while performing precision measurements of cosmic rays composition and flux. More than 110 billion charged cosmic ray events were collected by AMS-02. The AMS-02 observations will help answer fundamental questions, such as “What makes up the universe's invisible mass?” or “What happened to the primordial antimatter?” Anti-deuterons are a focus in the search for explanations to these questions. The unique sensitivity and long duration of the AMS-02 mission will allow researchers to measure the anti-deuteron flux for the first time and its conventional and dark matter components. Monte Carlo (MC) simulations are of vital importance for AMS-02 precision cosmic ray measurements, as they allow researchers to reliably compute the tiny details of the AMS-02 performance in space. This project will undertake MC simulations to optimize the winnowing of the dark matter signals from the massive amounts of data collected from the AMS-02.

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

Principal Investigator: Robert Voigt (Leidos Inc.)

Co-investigators:

S Balachandar (University of Florida)
Jonathan Freund (University of Illinois Urbana-Champaign)
Karel Matous (University of Notre Dame)
Gianluca Iaccarino (Stanford University)
Lawrence Rauchwerger (Texas A&M)
Martin Berzins (University of Utah)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 100,000,000 core-hours on Mira
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 78,500,000 core-hours on Titan
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 20,000,000 core-hours on Cori

Research Summary:

The Predictive Science Academic Alliance Program (PSAAP II) is a five-year program established in 2014 by the Advanced Simulation and Computing (ASC) program of the National Nuclear Security Administration to demonstrate predictive science in an extreme-scale computing environment. The PSAAP II research team will focus on a diverse set of complex applications of importance to DOE. This project will access the leadership computing facilities resources to demonstrate that the technologies and methodologies developed by these PSAAP II centers will effectively transition to extreme scale computing, simulating target applications with full physics and required resolution. The centers expect to gain insight into issues critical to the advancement to exascale computing, exposing areas where additional software research and development is needed.

Title: Multiphase Flow in Shale

Principal Investigator: David Trebotich (Lawrence Berkeley National Laboratory)

ALCC allocation:

Site: National Energy Research Scientific Computing Center (NERSC)

Allocation: 50,000,000 core-hours on Cori

Research Summary:

The objective of the DOE Energy Frontier Research Center for Nanoscale Control of Geologic CO₂ is to use new investigative tools to build a next-generation understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow and transport in porous rock media, in particular, as applied to geologic sequestration of CO₂. The overall goal of this project is to use direct numerical simulation at unprecedented scale and resolution to model pore scale processes associated with carbon sequestration and fracture evolution, in general, and to bring such knowledge to bear on the macroscopic scale of a reservoir.

Title: Imaging and Controlling Elemental Contrast of Nanocluster in Intense X-ray Pulses

Principal Investigator: Phay Ho (Argonne National Laboratory)

Co-investigators: Chris Knight (Leadership Computing Facility, Argonne National Laboratory)
Linda Young (Argonne National Laboratory)
Christoph Bostedt (Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 90,000,000 core-hours on Mira

Research Summary:

This project aims at a predictive understanding of the interaction of intense x-rays with complex nanoscale systems and to examine the potential applications of these x-rays. The ultrahigh intensity regime of x-ray interactions with matter was initiated with the advent of the Linac Coherent Light Source (LCLS) x-ray free-electron laser (XFEL). The achieved x-ray intensities can strip electrons from atoms from the inside out and create transient states of matter as the x-ray pulse progresses through the target. The goal of this project is to understand the impact of sample heterogeneity on the ultimate spatial resolution and elemental contrast achievable with XFEL pulses by examining the correlation of x-ray imaging with the induced dynamical processes on the most fundamental level. Using nanometer-sized heterogeneous clusters, particular attention is paid to the ultrafast electronic and nuclear ionization dynamics starting from ionization on the atomic level to charge transfer and electron redistribution within the sample, and the implications of the rapidly changing sample to the ultrafast x-ray scattering process. A hybrid quantum/classical simulation methodology will be used to investigate the interactions of intense XFEL pulses with nanometer-sized samples to understand the ultrafast dynamics and its connection to x-ray imaging and control. The work is an important step forward in understanding high-brightness, coherent x-ray laser pulses and their interactions with matter. The completion of the proposed work is essential in guiding the future XFEL experiments with heterogeneous materials and establishing the applied methodology as an effective large-scale computational tool for the new research frontier of ultrafast x-ray science.

Title: High-fidelity Numerical Simulation of Wire-wrapped Fuel Assemblies: Year 2

Principal Investigator: Aleksandr Obabko (Argonne National Laboratory)

Co-investigators:
Elia Merzari (Argonne National Laboratory)
Yiqi Yu (Argonne National Laboratory)
Landon Brockmeyer (Texas A & M University)

ALCC allocation:
Site: Argonne Leadership Computing Facility
Allocation: 83,500,000 core-hours on Mira

Research Summary:

Recent interest in advanced fuel cycles and reactor fuel recycling has led to renewed interest in the development of liquid-metal-cooled fast reactors in the United States. Several private companies have expressed interest in this technology, with a focus on cores with longer life. The prediction of thermal performance in fuel assemblies is vital for evaluating overall reactor performance and safety, particularly as the assembly ages. In particular, deformations driven by thermal expansion and radiation damage is increasingly important as reactor designs look to longer assembly lifetimes. As assemblies deform, traditional heuristic modeling becomes less suitable for evaluating the thermal-hydraulic performance of a given assembly due complex flow patterns that may be introduced. This project has the goal of validating higher fidelity tools to provide accurate predictions of the flow field and heat transfer in wire-wrapped fuel assemblies, typical of sodium fast reactor designs. The data obtained with these simulations will be instrumental in further improving lower-fidelity models and understanding the flow physics in this complex geometry. The present current work will carry out large eddy simulations of wire-wrapped fuel assemblies typical of liquid metal reactors with Nek5000 code for international benchmarks and fluid-induced vibration cases.

Title: Advances in Machine Learning to Improve Scientific Discovery

Principal Investigator: Robert Patton (Oak Ridge National Laboratory)

Co-investigators:
Thomas Potok (Oak Ridge National Laboratory)
Steven Young (Oak Ridge National Laboratory)
Catherine Schuman (Oak Ridge National Laboratory)
Travis Johnston (Oak Ridge National Laboratory)
Ramakrishnan Kannan (Oak Ridge National Laboratory)
Gabriel Perdue (Fermi National Accelerator Laboratory)

ALCC allocation:

Site: Oak Ridge Leadership Computing Facility
Allocation: 25,000,000 core-hours on Titan

Research Summary:

Scientific data sets have characteristics that differ substantially from traditional machine learning data sets. Machine learning methods have not been optimized to deal with these scientific data sets. Consequently, scientific data is often transformed and reduced in a way as to make it tractable for machine learning algorithms. However, much of the detail in the scientific data is lost in this transformation, likely sacrificing important insights embedded in the original data. This project focuses on extending machine learning tools to take advantage of the original data. The project will develop new computational approaches primarily based on convolutional and spiking neural network techniques to transform the original, non-reduced data sets in a more meaningful way and to understand deeper, spatiotemporal relationships in complex scientific data. In order to accomplish this task, the team will use use of high-performance computers to allow for large-scale model exploration to explore convolutional and spiking neural network models. If the project succeeds it will: 1) leverage more of the available scientific data in the analysis, and 2) push advanced analytic techniques closer to the point of data collection.

Title: Portable Application Development for Next Generation Supercomputer Architectures

Principal Investigator: T.P. Straatsma (Oak Ridge National Laboratory)

Co-investigators:
K.B. Antypas (Lawrence Berkeley National Laboratory)
T.J. Williams (Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 30,000,000 core-hours on Mira and 80,000,000 core-hours on Theta
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 30,000,000 core-hours on Titan

Research Summary:

This project will leverage computational resources at multiple supercomputing facilities to support the application readiness activities and portability studies necessary to prepare users for next generation computing architectures. ALCF, NERSC, and OLCF each run an early application readiness program that will prepare users for these next generation architectures. In order for the application readiness programs to be successful it is crucial that application developers have allocations not only at their sponsored supercomputing facility, but also at a facility with alternate architectures so that portability issues can be explored. The requested allocation will support the coordination and collaboration within these programs and provide resources to the application porting teams with the overall objective of delivering applications that are high performing and, as much as possible, architectural and performance portable.

Title: High-fidelity Simulations of Flow and Heat Transfer during Motored Operation of an Internal Combustion Engine

Principal Investigator: Paul Fischer (Argonne National Laboratory)

Co-investigators:

Ananias Tomboulides (Argonne National Laboratory)
Georgios Giannakopoulos (Swiss Federal Institute of Technology)
Christos Frouzakis (Swiss Federal Institute of Technology)
Misun Min (Argonne National Laboratory)
Saumil Patel (Leadership Computing Facility, Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)

Allocation: 30,000,000 core-hours on Theta

Research Summary:

Accurate, science-based simulations using computational fluid dynamics (CFD) can shed light on the complex phenomena within an internal combustion engine (ICE) by improving fundamental understanding that will help to establish and characterize the physical causes of stochastic events. This project will shed light on the complex phenomena and strongly-coupled processes inside an ICE by performing large-scale numerical simulations of a prototypical engine configuration. The approach will redefine the capability limits of high-fidelity simulations and will pave the way for detailed investigations of more complex phenomena in the future as computational power becomes increasingly available. Using Argonne's massively parallel computational fluid dynamics (CFD) code, Nek5000, this project will simulate the gas-exchange process over multiple cycles in the Transparent Combustion Chamber (TCC-III) engine for which extensive validation data are available from the University of Michigan. The project focus will be to investigate (a) the turbulent flow dynamics as the fluid passes through the moving intake valve during the intake stroke, (b) the evolution of the momentum and thermal boundary layers close to the cylinder walls, and (c) the impact of the turbulent flow motion on thermal stratification and local wall heat transfer. The simulations will be performed at the experimentally studied engine operating point of 800 revolutions per minute at full and part-load conditions. The results obtained with these highly accurate simulations will help clarify ambiguities in the interpretation of experimental measurements and will complement commercial codes for ICE simulation by providing best-in-class benchmark-type simulations.

Title: Impact of Grain Boundary Defects on Hybrid Perovskite Solar Absorbers

Principal Investigator: Wissam Saidi (University of Pittsburgh)

Co-investigators: Jin Zhao (University of Pittsburgh)
Alvaro Vázquez-Mayagoitia (Argonne Leadership Computing Facility)

ALCC allocation:
Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 20,000,000 core-hours on Mira

Research Summary:

Grain boundaries (GBs) are ubiquitous defects that can have profound effects on the mechanical and electronic properties of most polycrystalline materials. Although there have been significant improvements in experimental imaging and image analysis, it is still exceedingly difficult to unambiguously interpret the atomic structures within a GB region without well-established theoretical models for the interfaces. This challenge calls for the development of computational modeling approaches that can describe the GB region with high fidelity across the full five-parameter GB crystallographic space. This project will develop a multiscale approach to study GB structure, and apply the developed methodology to study the GB region and its properties in the methylammonium lead triiodide perovskites (MAPbI₃) that are of high interest for photovoltaics and optical applications. Here the project aims to develop and conduct a massively parallel, multiscale computational approach based on density functional theory and reactive force fields (RFFs) to determine the structure and properties of GBs. The research team will develop and use a genetic code to determine GB structure, investigate the properties of GB regions for defect segregation and their barriers at T=0K and room temperature, and develop a RFF for multicrystalline MAPbI₃.

Title: Emulating the Universe

Principal Investigator: Katrin Heitmann (Argonne National Laboratory)

Co-investigators:

Salman Habib (Argonne National Laboratory)
Andrew Hearin (Argonne National Laboratory)
Nicholas Frontiere (University of Chicago)
Esteban Rangel (Northwestern University)
Tom Uram (Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 10,000,000 core-hours on Mira
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 40,000,000 core-hours on Titan

Research Summary:

The aim of this project is the creation of a rich set of cosmological simulations, spanning different cosmological models to further our understanding of the make-up and history of the universe. Each cosmological simulation in the suite will be transformed into a synthetic sky that closely mimics actual observational data, allowing for a meaningful comparison with observations, including rigorous treatment of both theoretical and observational systematic errors. The project will use the simulation suite to build a set of high-accuracy prediction tools, so-called emulators. Emulators play an important role in the analysis of cosmological measurements. They allow the exploitation of the nonlinear regime of structure formation which holds important clues about the reason for the accelerated expansion of the universe. The simulations will be carried out with the Hardware/Hybrid Accelerated Cosmology Code, HACC. HACC was designed to take full advantage of contemporary and future hardware architectures. For this project, researchers will run HACC on two completely different supercomputer architectures, the BG/Q Mira at the Argonne Leadership Computing Facility and the GPU-enhanced system at Oak Ridge Leadership Computing Facility. The final aim is to make products from the simulation campaign available to the cosmology community to extend the science reach of these unique simulations even further.

Title: Petascale Analytics of Big Proteogenomics Data on Key Microbial Communities

Principal Investigator: Chongle Pan (Oak Ridge National Laboratory)

Co-investigators: Melanie Mayes (Oak Ridge National Laboratory)
Hassan Brim (Howard University)

ALCC allocation:
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 50,000,000 core-hours on Titan

Research Summary:

Proteogenomics measurements reveal the genomic sequences and enzyme inventories of microbial communities. This information provides valuable insights into biological processes in microbial ecosystems and their responses to different environmental perturbations. The increased throughput in sequencing and mass spectrometry technologies enabled the generation of big proteogenomics data to achieve more comprehensive coverage of complex microbial communities across a large number of environmental conditions. This project will use our scalable proteogenomics data analytics capabilities and the Titan supercomputer for studies of plant rhizosphere communities, tropical soil communities, and human gut microbiota.

Title: HPC4EnergyInnovation ALCC End-Station

Principal Investigator: Peter Nugent (Lawrence Berkeley National Laboratory)

Co-investigators: Lin-Wang Wang (Lawrence Berkeley National Laboratory)
Debbie Bard (Lawrence Berkeley National Laboratory)
Robert Saye (Lawrence Berkeley National Laboratory)
Jane McFarlane (University of California Berkeley)
Scott Roberts (Sandia National Laboratories)
Srikanth Allu (Oak Ridge National Laboratory)
Ramanan Sankaran (Oak Ridge National Laboratory)
David Pointer (Oak Ridge National Laboratory)
James Morris (Oak Ridge National Laboratory)
Prashant Jain (Oak Ridge National Laboratory)
John Turner (Oak Ridge National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 20,000,000 core-hours on Theta
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 100,000,000 core-hours on Titan
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 50,000,000 core-hours on Cori

Research Summary:

For the past two years the HPC4Mfg program has united the world-class high performance computing resources and scientific expertise at the DOE national laboratories with U.S. industry to advance revolutionary manufacturing solutions. This program has now branched out across the DOE/EERE mission space to include programs in Materials (HPC4Mtls) and Vehicle Technology and Mobility (HPC4Mobility). This ALCC End-Station project, entitled HPC4EnergyInnovation, will provide the HPC time necessary to fulfill the goals of these individual projects. This allocation will advance the adaptation of advanced HPC codes into powerful tools for applied energy innovation for manufacturing, mobility, and materials applications.

Title: Investigating the Impact of Improved Southern Ocean Processes in Antarctic-focused Global Climate Simulations

Principal Investigator: Mark Petersen (Los Alamos National Laboratory)

Co-investigators:
 Xylar Asay-Davis (Los Alamos National Laboratory)
 Darin Comeau (Los Alamos National Laboratory)
 Matthew Hoffman (Los Alamos National Laboratory)
 Stephen Price (Los Alamos National Laboratory)
 Luke Van Roekel (Los Alamos National Laboratory)
 Phillip Wolfram (Los Alamos National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 35,000,000 core-hours on Theta
Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 5,000,000 core-hours on Titan
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 65,000,000 on Edison

Research Summary:

Despite its distance from human settlement, the Antarctic is a critical region for assessing global effects of climate change. The Southern Ocean covers less than one third of the global ocean but dominates the ocean's ability to absorb carbon dioxide and heat and mitigate climate change. The expansive sea ice surrounding Antarctica and the deep cavities beneath the continent's fringing ice shelves are the planet's biggest factories of dense ocean bottom water that helps drive global ocean circulation. Interactions of the Southern Ocean with the Antarctic Ice Sheet are driving rapid melting of the ice shelves that restrain the grounded ice behind them and potential collapse of parts of the ice sheet, which in turn would result in significant sea level rise—potentially up to a meter by 2100—with disruption or displacement of 40% of the world's coastal populations. Projecting future sea level rise from Antarctica using a global, coupled Earth System Model that realistically simulates the Southern Ocean is one of three primary science drivers of the Department of Energy's Energy Exascale Earth System Model (E3SM) project. The E3SM climate simulations span from a historical twentieth century climate to the present and into the next century with several emissions scenarios. This project will study: the natural climate variability of sub-ice shelf melt rates; changes in melt rates over time and with future scenarios; and the influence on regional Antarctic climate of eddy dynamics, ocean vertical mixing, iceberg calving, changing ocean currents, reduced sea ice cover, and changes in ice shelf geometry.

Title: Simulations of Laser Experiments to Study MHD Turbulence and Non-thermal Charged Particles

Principal Investigator: Petros Tzeferacos (University of Chicago)

Co-investigators:

Don Lamb (University of Chicago)
Scott Feister (University of Chicago)
Norbert Flocke (University of Chicago)
Benjamin Khier (University of Chicago)
Klaus Weide (University of Chicago)
Carlo Graziani (Argonne National Laboratory)
Katherine Riley (Argonne National Laboratory)
Venkatram Vishwanath (Argonne National Laboratory)

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 22,000,000 core-hours on Mira

Research Summary:

Magnetic fields are ubiquitous in the universe. The standard theoretical model behind their origin is the amplification of tiny seed fields via turbulent dynamo, resulting in turbulent magnetized plasmas. These turbulent plasmas mediate the propagation and acceleration of non-thermal charged particles via scattering and second-order Fermi acceleration—a stochastic process whereby cosmic rays gain energy through scattering with randomly moving magnetized clouds. This project has both experimental and simulation thrusts. The experiments are designed to study the properties of magnetized turbulent plasmas and non-thermal particles in the laboratory. The project has been awarded shot-time at both the Omega laser facility at the Laboratory for Laser Energetics at the University of Rochester, and the National Ignition Facility at Lawrence Livermore National Laboratory. These extremely powerful lasers allow researchers to produce magnetized turbulence at large magnetic Reynolds numbers, which is required for the nonlinear turbulent dynamo mechanism to occur. The experiments are designed and interpreted using validated simulations performed with the radiation-MHD code, FLASH; the FLASH simulations are vital to ensure the experiments achieve the desired flow properties. This project will undertake 3D FLASH simulations to capture the properties of the turbulence, and resolve the small spatial scales at which amplification occurs. FLASH simulations are also critical in determining the timing of experiment diagnostics, since the signals last only a few nanoseconds, and the interpretation of the experimental results.

Title: Molecular Simulation in Bioenergy and Biomedical Sciences

Principal Investigator: Jeremy Smith (Oak Ridge National Laboratory)

ALCC allocation:

Site: National Energy Research Scientific Computing Center (NERSC)

Allocation: 10,000,000 core-hours on Edison

Research Summary:

Molecular simulation can play a critical role in the rational design of biosystems. This project will undertake molecular design studies targeting bioenergy research as well as biomedical applications. The latter represents a relatively new direction of the DOE that wishes to apply techniques mastered in the national laboratories to problems of interest to the NIH. High-performance computing will be employed to design peptide-based vaccines. This project involves the design of a vaccine against Group A Streptococcus bacteria. Furthermore, researchers will perform computer simulations of neoantigen binding to the Major Histocompatibility Complex with a view to selecting antigens for cancer vaccines.

Title: Large Scale Numerical Simulations of Polymer Nanocomposites

Principal Investigator: Gary Grest (Sandia National Laboratories)

Co-investigators: Shengfeng Cheng (Virginia Polytechnic Institute and State University)
Sanat Kumar (Columbia University)
Dvora Perahai (Clemson University)
Michael Rubinstein (Duke University)

ALCC allocation:

Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 8,000,000 core-hours on Titan
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 20,000,000 core-hours on Cori and 45,000,000 core-hours on Edison

Research Summary:

The pathways to control assembly and integration of nanoparticles into polymeric matrices will be probed using multi-million atom molecular dynamics simulations. The potential of nanoparticles has been long realized. However, integrating them in different devices remains a challenge. This study will probe ways to overcome the major barriers to integrating nanoparticles into a range of advanced devices, controllably dispersing and organizing them within durable matrices while retaining their unique properties. By zooming into the interaction regions between the nanoparticles and the surrounding polymeric matrix, this project will provide the needed molecular level understanding of the assembly process. Specifically, researchers seek to resolve the factors that control the assembly of multiple nanoparticles in bulk and in thin films. As producing well-dispersed polymer nanocomposites is a major hurdle for making new materials, studies will concentrate on identifying the parameters that control dispersion. It is then possible to determine the rheological response and mechanical properties of the resulting polymer nanocomposites and study molecular transport through polymer nanocomposite membranes for gas separation.

Title: Steady State Engine Calibration in CFD using a GPU-based Chemistry Solver, Conjugate Heat Transfer, and Large Eddy Simulation (LES)

Principal Investigator: Ronald Grover (General Motors)

Co-investigators:

Jian Gao (General Motors)
Venkatesh Gopalakrishnan (General Motors)
Ramachandra Diwakar (General Motors)
Wael Elwasif (Oak Ridge National Laboratory)
K. Dean Edwards (Oak Ridge National Laboratory)
Charles Finney (Oak Ridge National Laboratory)
Russell Whitesides (Lawrence Livermore National Laboratory)
Keith Richards (Convergent Science)

ALCC allocation:

Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 12,000,000 core-hours on Titan

Research Summary:

The research team of General Motors, Oak Ridge National Laboratory, Lawrence Livermore National Laboratory, and Convergent Science has been developing a highly detailed model of a light-duty diesel engine. The team is developing the model in CONVERGE™ by systematically replacing simplified submodels with more predictive approaches based on first principles and evaluating the resulting impacts on computational requirements and accuracy compared with experimental engine performance and emissions data. This project will extend earlier studies by adding a Large Eddy Simulation turbulence model in conjunction with detailed kinetics, refined grid, and conjugate heat transfer. The final model will be one of the most complex, detailed engine simulation tools developed in the open literature and will help to define industry best practices in detailed engine simulation.

Title: Phase Boundary of Baryon-rich QCD Matter

Principal Investigator: Swagato Mukherjee (Brookhaven National Laboratory)

Co-investigators:

F. Karsch (Bielefeld University, Germany)
A. Bazavov (Michigan State University)
H.-T. Ding (Central China Normal University, China)
R. Larsen (Brookhaven National Laboratory)
P. Petreczky (Brookhaven National Laboratory)
P. Steinbrecher (Brookhaven National Laboratory)

ALCC allocation:

Site: Oak Ridge Leadership Computing Facility (OLCF)
Allocation: 85,000,000 on Titan at OLCF, and
Site: National Energy Research Scientific Computing Center (NERSC)
Allocation: 125,000,000 core-hours on Cori

Research Summary:

The transition temperature of the strong-interaction matter, described by the theory of Quantum Chromodynamics (QCD), is one of the fundamental scales within the Standard Model of physics, and tells us about the thermal condition when the universe transitioned from quark-gluon soup to the nuclear matter present today. Using state-of-the-art lattice QCD computations, this project seeks to determine the transition temperature of strong-interaction matter containing more baryons than antibaryons and, thereby, delineate the phase boundary of baryon-rich QCD matter in the temperature and baryon chemical potential plane. These results will not only enhance our fundamental knowledge about strong-interaction matter but also guide the experimental explorations of the QCD phase diagram, particularly the Beam Energy Scan (BES) program at the Relativistic Heavy Ion Collider (RHIC). Additionally, these lattice QCD calculations will provide many other urgently needed QCD inputs that are essential for dynamical modeling of RHIC's BES.

Title: Nucleon Structure and Electric Dipole Moments with Physical Chiral-symmetric Quarks

Principal Investigator: Sergey Syritsyn (RIKEN BNL Research Center)

Co-investigators:

Michael Engelhardt (New Mexico State University)
Jeremy Green (NIC, Deutsches Elektronen-Synchrotron, Germany)
Taku Izubuchi (RIKEN BNL Research Center)
Christos Kallidonis (Stony Brook University (SUNY))
Meifeng Lin (Brookhaven National Laboratory)
John Negele (Massachusetts Institute of Technology)
Hiroshi Ohki (Department of Physics, Nara Women's University, Japan)
Shigemi Ohta (RIKEN, Japan)
Andrew Pochinsky (Massachusetts Institute of Technology)
Jun-Sik Yoo (Stony Brook University (SUNY))

ALCC allocation:

Site: Argonne Leadership Computing Facility (ALCF)
Allocation: 50,000,000 core-hours on Mira

Research Summary:

Our project aims at understanding the internal structure of the proton and neutron by numerical solution of Quantum Chromodynamics, the fundamental theory governing their constituents, quarks and gluons. Protons and neutrons (collectively called nucleons) are the basic building blocks of ordinary matter. Their internal dynamics is far from clear: e.g., distributions of their charge and magnetization, the origin of their mass and spin, and even the proton radius are now under question. Experiments at Jefferson Lab and the Relativistic Heavy Ion Collider (RHIC) study these questions, and our project will address them using fundamental theory. Nucleons also serve as a gateway for modern experiments searching for yet undiscovered particles and interactions that may explain, among other things, the mysterious Dark Matter and the incredibly small masses of neutrinos. Nucleons were created shortly after the Big Bang, but we do not understand why this baryogenesis produced far more nucleons than antinucleons - a key prerequisite for our existence. Some fundamental symmetries have to be violated more strongly than current particle physics can accommodate, and searches for these violations are among the most important goals of the DOE nuclear physics program. In particular, the so-called charge conjugation parity symmetry (CP symmetry) violations are searched for in measurements of permanent electric dipole moments of nucleons and nuclei. Two such experiments on the US soil are expected to start gathering data by 2020. Interpreting results of these experiments will depend critically on reliable knowledge of nucleon structure, and this project will further our theoretical knowledge using the most realistic calculations feasible today.