U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Scale-Aware Modeling of Instabilities and Mixing in HED Flows

Principal Investigator: Hussein Aluie, University of Rochester

Co-Investigators:

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
30,000 node hours

Research Summary

Instabilities and mixing are detrimental to system performance in high-energy density (HED) applications such as fusion power systems. Numerical models used in HED applications have had significant difficulties predicting the instabilities and mixing that occur in experiments. Most of these "global- system" models cannot resolve a sufficient level of vorticity that develops hydrodynamically. Recent evidence from several independent investigations indicates that this shortcoming contributes to under- predicting the levels of instability growth and mixing in such highly nonlinear flows. Routinely conducting multi-physics global-system three-dimensional simulations at the high resolution required to resolve the missing vorticity is not feasible in the foreseeable future due to the exorbitant computing cost. To address this problem, we have utilized a novel "coarse-graining" scale-analysis approach that is versatile and powerful to develop a nonlinear mixing model (NMM) capable of accounting for the missing vorticity in a self-consistent manner. Coarse-graining has a rigorous mathematical foundation and is closely related to well- established physics techniques, including macroscopic electromagnetism, renormalization group, and Large Eddy Simulations. NMM is a deterministic model of vorticity and strain that is "scale-aware" in the sense that it self-adjusts to the underlying numerical resolution without relying on user input. NMM is also portable in the sense that it is not dependent on a particular numerical scheme and can be eventually deployed in HED application codes. With these eventual goals in sight, this proposal aims to test and validate the NMM using our codes by relying on high-resolution simulations.

The project should enable HED application codes, such as those used in fusion, to better predict instability growth and mixing at a significantly lower computational cost.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Enabling Resilient and Portable Workflows from DOE's Experimental Facilities

Principal Investigator: Katerina Antypas, Lawrence Berkeley National Laboratory

Co-Investigators: Debbie Bard, Lawrence Berkeley National Laboratory,
Tom Uram, Argonne National Laboratory,
Venkat Vishwanath, Argonne National Laboratory,
Mallikarjun Shankar, Oak Ridge National Laboratory,
Suhas Somnath, Oak Ridge National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Oak Ridge Leadership Computing Facility (OLCF)
20,000 node hours

Research Summary

The size and complexity of data from DOE's experimental and observational facilities is already overwhelming scientists' ability to manage, analyze, search and model it. Data set sizes are expected to grow dramatically in the next decade. As a result, scientists from these facilities are increasingly turning to HPC for their workloads including large scale data analysis, AI, and simulation and modeling. These workflows often have different requirements from traditional simulation workloads based on their need for near real-time feedback, experiment-time availability, and resilience. HPC Facilities are optimized for high utilization and large-scale jobs. Further, the first-of-a-kind technologies deployed at ASCR HPC facilities requires a period of hardening before systems reach full stability. Once in production, downtimes are necessary for repairs and upgrades that can again affect stability. Resolving this impedance mismatch requires creative and innovative solutions to provide resilience for complex workflows originating from DOE's experimental and observational facilities. There have been many efforts to address application portability, which primarily focus on portable programming models and node architectures. More research and experimentation is needed to enable portable complex cross-facility workflows that would enable a new generation of facilities. This project will enable research into the unique challeges from experimental and observational data workloads for HCP facilitites. With some adaptation, EOD applications have been run at large scale across the DOE complex. Notable examples include simulation from high energy physics and astrophysics, and analysis of data from DOE light sources. One goal of this project will be to generalize these successes to other applications and domains. A second goal will be to prototype flexibility in scheduling jobs across the compute facilities. This portability will be explored in the context of workloads from partner DOE facilities. Ultimately, this work will define the architectural and technical roadmap for experimental and observational facility workflows running on ASCR HPC facilities, expose the cross-facility policy challenges, and offer strategies to address them.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: High Luminosity LHC detector upgrade studies by the ATLAS and CMS collaborations

Principal Investigator: Douglas Benjamin, Argonne National Laboratory

Co-Investigators: Dirk Hufnagel, Fermi National Accelerator Laboratory (co-PI);
Paolo Calafiura, Lawrence Berkeley National Laboratory;
Eric Lancon, Brookhaven National Laboratory;
Oliver Gutsche, Fermi National Accelerator Laboratory;
Tulikla Bose, University of Wisconsin-Madison;
James Letts, University of California San Diego

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
950,000 node hours

National Energy Research Scientific Computing Center (NERSC)
250,000 node hours

Research Summary

In July 2012, the Higgs Boson was discovered at the Large Hadron Collider (LHC) at CERN (Switzerland) by both the ATLAS and CMS collaborations.

The ATLAS and CMS collaborations are in the process of writing Technical Design Reports associated with High Luminosity-LHC (HL-LHC) upgrades to both the detectors and the trigger – data acquisition system. A significant amount of simulated data is required in preparation for these reports. This data will need to be produced across a wide range of HL-LHC beam conditions. The HL-LHC simulated events are much more complex compared to current simulated data. Many parts of the ATLAS and CMS HL-LHC detectors will be new and new reconstruction algorithms will need to be developed. The simulated data samples produced from this ALCC allocation will be highly valuable for the collaborations and instrumental in the development of new reconstruction algorithms. This simulated data will be produced using both parameterized models and Geant4 simulation software and digitized/reconstructed if necessary. This software has been used at both NERSC-Cori and ALCF-Theta by both collaborations.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Multiphase Flow Simulations of Reactor Flows

Principal Investigator: Igor Bolotnov, North Carolina State University

Co-Investigators: Jun Fang, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
192,000 node hours

Research Summary

The proposed ALCC project will capitalize on existing multiphase flow experience to utilize interface capturing methods and direct numerical simulation to perform state of the art large scale simulations of reactor flows. PHASTA code has a long history of HPC performance, and our group has been awarded 2014, 2016 and 2018 ALCC awards in the past advancing the mission of DOE. PHASTA is a finite-element based flow solver with level-set method for interface capturing approach. It utilizes unstructured meshes and has been shown to scale very well on Theta ANL machine.

The project will include 2 subprojects: (i) full scale simulation of table-top bubbly plasma generator and (ii) heat transfer simulation of turbulent flows of novel coolants for advanced nuclear reactor models development. These represent a novel simulation of a single- and two-phase flows which has not been done before at the proposed conditions and computational scale.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Multiscale edge turbulence in fusion plasmas

Principal Investigator: Jeff Candy, General Atomics

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
56,000 node hours

Research Summary

A one-year focused project is proposed to exploit the leadership-scale edge-plasma turbulence simulation capabilities of CGYRO. A relatively new code, CGYRO was recently designed from the ground up in order to simulate the edge region of fusion tokamak plasmas using numerical methods tailored to modern multicore and GPU architectures. A key distinguishing feature of this work is to operate at true multiscale resolution with full ion-electron coupling.

In the edge region of a fusion plasma, direct numerical simulation of turbulence is challenging due to strong density and temperature gradients and extreme cross-sectional plasma shaping. One particular edge config- uration, the so-called H-mode, is the most promising scenario envisioned to achieve controlled nuclear fusion in tokamaks. An H-mode features a narrow region (pedestal) just inside the magnetic boundary (separatrix) where strong plasma flows can reduce the turbulence intensity. The low levels of edge turbulence cause the steep pedestal structure which substantially increases the core density and temperature.

The proposed work will serve to refine theoretical understanding of the pedestal and provide a database of results in order to calibrate the TGLF (the GA turbulent transport model).

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Improving Direct-Drive Laser Fusion Predictive Capability with a Simulation Database

Principal Investigator: Duc Cao, Laboratory for Laser Energetics, LLE, University of Rochester

Co-Investigators: P. B. Radha Laboratory for Laser Energetics, LLE, University of Rochester

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
318,000 node hours

Research Summary

Large-scale simulations of direct-drive Inertial Confinement Fusion (ICF) implosions are proposed for the ALCC allocation. These simulations model experiments on the OMEGA laser, where a spherical cryogenic layer of deuterium-tritium enclosed in a thin polymeric shell is imploded to produce neutrons. Many measurements are made on each implosion to study its performance. The goal of these implosion experiments is to improve performance such that Mega-Joule-type fusion yields would be possible when scaled to the National Ignition Facility (NIF).

These simulation studies proposed through the ALCC program can significantly impact the direct-drive ICF program. They will potentially help identify dominant sources of nonuniformity, mitigation of which will lead to improved target performance. They will also help identify target designs in which nonuniformity might have a reduced impact on target performance. With improved performance in direct-drive implosions on OMEGA (a kilojoule class laser), ICF has the potential for ignition on Mega-Joule class lasers (such as the NIF). These types of improved implosions are also relevant on platforms to study many different applications related to national security and other fields of physics including nuclear astrophysics and material properties under strongly coupled and degenerate conditions.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Nonlinear Rheology of Entangled Polymers

Principal Investigator: Jan Michael Carrillo, Oak Ridge National Laboratory

Co-Investigators: Wei-Ren Chen, Oak Ridge National Laboratory
Yangyang Wang, Oak Ridge National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
183,000 node hours

Research Summary

The flow and deformation of macromolecules is ubiquitous in nature and industry, and an understanding of this phenomenon in both macroscopic and microscopic length scales is of fundamental and practical importance. Every year, several hundred billion pounds of polymers are consumed to make commercial rubber and plastic products. Many of these processes involve entangled polymers, chain-like molecules sufficiently long such that the motion of a chain is constrained by those of its neighboring molecules, which leads to perplexing nonlinear flow behavior. The proposed study aims at pushing the boundary of our understanding of the nonlinear rheological behavior of entangled polymers by using large-scale molecular dynamics simulation.

The objective of the proposed large-scale molecular dynamics simulation work is to perform a comprehensive microscopic investigation of the conformational changes of well-entangled polymers under flow and deformation, using a novel conceptual framework that brings together analytical theories, molecular simulations, rheology, and small-angle neutron scattering experiments. The specific aims of our research include: (1) Examine classical models by analysis of spatial dependence of configuration distribution, (2) Reveal microscopic deformation mechanism by studying the time evolution of spatially-dependent structural functions, and (3) Establish the universal underlying physics governing the nonlinear rheology of entangled polymers.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Data-driven Molecular Engineering of Advanced Functional Materials

Principal Investigator: Jacqueline Cole, University of Cambridge

Co-Investigators: Álvaro Vázquez-Mayagoitia, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

The world needs new materials to stimulate the chemical industry in key sectors of our economy: environment and sustainability, information storage, and optical sensing. Yet, nearly all functional materials are still discovered by 'trial-and-error', whose lack of predictability affords a major materials bottleneck to technological innovation. The emerging field of data-driven molecular engineering offers a prospective solution to this problem. It enables systematic molecular design and engineering strategies to be encoded into algorithms that search through massive chemical datasets, and couple with computational workflows, to discover a material that suits a bespoke application. Such data-science approaches to materials discovery are only just becoming possible, given recent advances in artificial intelligence, rapid rises in high-performance-computing, and changes in government legislation that regulates open-access of scientific data. The US government promotes this approach via the Materials Genome Initiative, which aims to reduce the average 20 year 'molecule-to-market' timeframe in industry.

This ALCC project will develop data-driven materials-by-design capabilities to accelerate the discovery of new materials for photovoltaic and quantum optical sensing applications.

We will achieve our goal by exploiting the latest advances in materials database auto-generation tools and data-mining, which harness artificial intelligence and machine learning. These have been developed by the Molecular Engineering group at Cambridge, UK. They have facilitated the group's award-winning materials discovery capabilities through rational molecular design and experimental validation. This ALCC project will extend a partnership between the Molecular Engineering group at Cambridge and Argonne National Laboratory (ANL), where they have been already collaborating in computation and data-science, at the Argonne Leadership Computing Facility (ALCF) since 2016, and experimentally, at the Advanced Photon Source (APS) and the Center of Nanoscale Materials (CNM) since 2013.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Variable Resolution Earth System Modeling of the Cryosphere with E3SM

Principal Investigator: Darin Comeau, Los Alamos National Laboratory

Co-Investigators: Xylar Asay-Davis, Los Alamos National Laboratory,
Matthew Hoffman, Los Alamos National Laboratory,
Mark Petersen, Los Alamos National Laboratory,
Stephen Price, Los Alamos National Laboratory,
Andrew Roberts, Los Alamos National Laboratory,
Wuyin Lin, Brookhaven National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
400,000 node hours
National Energy Research Scientific Computing Center (NERSC)
500,000 node hours

Research Summary

Antarctica and the Southern Ocean play critical roles in modulating global climate and sea level. While their response to climate change is among the least understood in the climate system, the potential global ramifications are among the most severe. The Antarctic ice sheet holds many tens of meters of sea-level equivalent, and ice shelves directly exposed to the ocean are integral to restraining the grounded ice behind them. Increased melting of ice shelves could cause collapse of parts of the ice sheet, leading to rapid sea level rise that may displace low-lying coastal populations and threaten coastal infrastructure worldwide.

Despite its importance, the Antarctic ice sheet and its interactions with the Southern Ocean remain poorly represented in most Earth system models. One of three primary science drivers for the DOE's Energy Exascale Earth System Model (E3SM) is to realistically simulate coupled Antarctic and Southern Ocean processes, towards allowing for projections of Antarctica's contribution to future sea-level rise.

This project will enable development, testing, and simulations of the E3SM v2 Cryosphere campaign. This includes scientific investigations into how the coupled atmosphere, ocean, and sea-ice system will mediate current and future sources of sea-level rise from the Antarctic ice sheet. A general focus of E3SM v2 is the utilization of its unstructured variable resolution capability. To that end, the proejcet team is developing and testing regionally refined coupled Southern Ocean configurations for the ocean, sea-ice, and atmosphere.

Another E3SM capability at the forefront of Earth system modeling is the ability to simulate ocean circulation under Antarctic ice shelves, allowing the compututation of melt rates from these ice shelves in global, fully coupled configurations. These melt rates are a key source of uncertainty in future sea-level rise. Because sea-ice plays a key role in moderating the water masses that access ice shelf cavities, part of this effort will focus on improvements to sea-ice physics and coupling numerics to mitigate low resolution (30km) ice extent biases and high resolution (6km) ice thickness biases in E3SM version 1.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Proton quasi-PDFs and quasi-GPDs from lattice QCD

Principal Investigator: Martha Constantinou, Temple University

Co-Investigators: Constantia Alexandrou, University of Cyprus & The Cyprus Institute

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

The theory of the strong interactions, Quantum Chromodynamics (QCD), binds permanently quarks into hadrons, giving them rich and complex structure. Understanding their structure from first principles requires a systematic and quantifiable study of QCD, as fundamental properties of the hadronic matter arise from the Standard Model and QCD dynamics. At the hadronic energy scales, solution of QCD is not amenable to perturbation theory. The only non-perturbative approach that captures the full QCD dynamics is a discretization of the continuum theory on a 4-dimensional Euclidean lattice for numerical simulations on powerful computers. This approach, known as lattice QCD (LQCD), provides a rigorous framework for studying hadron structure non-perturbatively starting directly from the underlying fundamental theory.

With this ALCC request for computer allocation, we propose several improvements of our research program on quasi-PDFs, as well as, a novel calculation of quasi-GPDs which complement TMDs in the study of the 3-D structure of hadrons. We will compute the unpolarized, helicity, and transversity quasi-PDFs, and explore quasi-GPDs. The quasi-distribution approach requires matrix elements with fast-moving hadrons, and we will study the momentum dependence. Moreover, we will investigate new lattice techniques for the calculation of the disconnected contributions of non-local operators. This direction has never been explored so far and will open new avenues for the extraction of PDFs for individual quarks within the proton.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Precision Lattice QCD for Flavor Physics

Principal Investigator: Carleton DeTar, University of Utah

Co-Investigators: Thomas Blum, University of Connecticut
Luchan Jin, University of Connecticut
Norman Christ, Columbia University
Kate Clark, NVIDIA
Aida El Khadra, University of Illinois
Zechariah Gelzer, University of Illinois
Elvira Gámiz, University of Granada
William Jay, Fermi National Accelerator Laboratory
Chulwoo Jung, Brookhaven National Laboratory
Andreas Jüttner, Southampton University

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

The search for new physics beyond the Standard Model of elementary particles is a major goal of contemporary high energy physics and is one of the top five science drivers listed by the 2014 DOE P5 report. We propose to increase significantly the accuracy of the Standard Model predictions in two related areas with particularly promising discovery potential.

We are using methods of lattice quantum chromodynamics to reduce the error on the predicted value for the anomalous magnetic moment of the muon, g_μ-2, arising from hadronic vacuum polarization to 1% or smaller. We plan two complementary efforts using two lattice-quark formulations with different systematic uncertainties, namely, the highly-improved-staggered-quark and the domain-wall-fermion methods. We will harness the power of Summit to extend earlier calculations to smaller lattice spacing and lattice volumes as large as 96^3 x 192, giving increased control of systematic discretization errors. We will also carry out the first physical-mass calculation of the indirect charge-parity -violation parameter of ε_k. This will be done on a 64^3 x 128 lattice volume using all-to-all propagators for four-quark-operator self contractions and include nonperturbative renormalization of the bilocal, second-order weak operator that enters. All of these calculations involve increasingly mature Summit code running on partitions of between 64 and 1024 nodes. These calculations are accelerated by low-mode deflation with as many as 5000 eigenvectors per configuration.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Field-Reversed Configuration Stability and Transport

Principal Investigator: Sean Dettrick, TAE Technologies, Inc

Co-Investigators: Francesco Ceccherini, TAE Technologies, Inc,
Calvin Lau, TAE Technologies, Inc,
Toshiki Tajima, UC Irvine

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
64,000 node hours

National Energy Research Scientific Computing Center (NERSC)
26,000 node hours

Research Summary

TAE Technologies, Inc (TAE) has developed an advanced beam-driven Field-Reversed Configuration (FRC) for magnetic confinement of fusion plasmas, with the goal to develop a commercially viable source of electricity based on aneutronic nuclear fusion using the proton-Boron-11 fuel cycle. On our current experimental device named Norman, aka C-2W, we have demonstrated the capacity to sustain high temperature, stable, long-lived FRC plasmas by a combination of compact-torus (CT) collision, Neutral Beam (NB) injection and edge biasing.

This project will provide theory support for the existing C-2W fusion plasma experiment at TAE. It will also contribute to the current effort to design our next-step FRC device, which will be known as Copernicus. Copernicus will be a reactor-scale prototype designed to demonstrate the ability to achieve fusion relevant conditions in the early 2020s.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Distributed large wavefield propagation and 3D reconstruction beyond the depth of focus limit

Principal Investigator: Ming Du, Advanced Photon Source, Argonne National Laboratory

Co-Investigators: Chris Jacobsen, Advanced Photon Source, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
250,000 node hours

Research Summary

X-ray microscopy is unique in combining the potential for nanoscale spatial resolution with the ability to image samples up to centimeters thick. The $800M upgrade of the Advanced Photon Source (APS) will increase beam brightness more than 100x, allowing one to fully realize this potential. However, a fundamental challenge remains: as one improves (decreases) the spatial resolution, the depth of focus of imaging decreases. This means that the beam profile may undergo significant variation when a thick sample is imaged, which violates the standard approximation that a 2D image is a pure projection through a 3D object. This challenge is not yet widely appreciated in x-ray microscopy, but if unmet it will present severe limitations to fully exploiting the capabilities of the APS Upgrade.

This project willl model the diffraction of X rays in an object variable using the multislice method, which predicts the detected wavefield intensity downstream the sample. The object function is then iteratively updated using a gradient-based approach, so that the data mismatch between the prediction and the experimental measurement (i.e., the loss function) is minimized with an ultimate goal of nanometer resolution in centimeter-sized samples. The project will also implement parallelized wave propagation modeling and reconstruction approaches that are more efficient for large samples, and compare their results. With experimental data planned to be collected in 2020, we will validate our algorithm in real-world scenarios.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Confronting the New Challenges in Hadron Spectroscopy

Principal Investigator: Robert Edwards, Thomas Jefferson National Accelerator Facility

Co-Investigators: Balint Joo, Thomas Jefferson National Accelerator Facility

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

Hadrons are the particles of which the atomic nucleus is made. While protons, neutrons and pions are the best known of these, hundreds of hadrons have been observed. These can be grouped into families: baryons, including the proton, and mesons, of which the pion is the lightest. These hadrons are in turn built of more fundamental objects, namely quarks in different varieties, or flavors. Quarks are bound together to make each hadron by a strong force that is mediated by gluons, and is well described by the equations of Quantum Chromodynamics (QCD). All the known baryons can be constructed from three quarks, while mesons are built of a quark and an antiquark, each in their different flavors. Protons and pions are made of the lightest quarks, known as up and down. Together with strange quarks, these make up the light quark sector.

Recent discoveries of unexpected states in the heavy quark sector, and tantalizing suggestions of unexpected states in the light quark sector, have ignited a firestorm of activity. The GlueX experiment of the new Hall D at the Thomas Jefferson National Accelerator Facility (Jefferson Lab), a flagship component of the $338 million upgrade of Jefferson Lab, has a primary purpose to provide a detailed description of putative "exotic'' mesons.

These states are expected to provide the most direct evidence of new configuration of matter, where gluonic degrees of freedom are manifest, known as "hybrids".

Recent experiments at the LHC (CERN), BELLE (SLAC) and BES (Beijing), have presented evidence of unexpected states in the heavy quark sector -- including suggestions of charm and light quark configurations forming tetraquarks. The LHCb experiment has suggested evidence for pentaquarks. These configurations do not fit into the conventional description of matter in the prevailing view of hadronic physics.

This proposal is timely: we will provide first direct confrontation of the existence of possible tetraquark states in QCD as well as exotic mesons in the light quark sector. The predictions for the decay rates of these putative particles will confront and guide experiments, including the GlueX experiment at Jefferson Lab. The importance of these searches has been emphasized in the most recent report to the DOE Nuclear Science Advisory Committee for the 2015 Long Range Plan: "Underscoring this huge progress, LQCD plays an essential role in guiding experimental work. GlueX at JLab, one of the flagship experiments of the 12-GeV Upgrade, is designed to search for exotic particles where the glue is in an energetically excited state. Initial LQCD calculations motivated the experiment and guided its design. Recent LQCD results confirm the mass range of the predicted particles. And in the future, LQCD calculations of hadron dynamics will play a critical role in the analysis of the data."

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Quantum Turbulence in Fermi Superfluids

Principal Investigator: Michael Forbes, Washington State University

Co-Investigators: P. Magierski, Warsaw University of Technology
G. Wlazlowski, Warsaw University of Technology

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
300,000 node hours

Research Summary

Turbulent phenomena abound in nature, playing a vital part in the dynamics of the wide variety of classical fluids on scales ranging from millimeters to light years. Indeed they can be found in the interior of biological cells, in circulatory and respiratory systems of living creatures, in countless technological devices, and in astrophysics where turbulence appears in planetary interiors, oceans and atmospheres, and even on galactic scales. Quantum turbulence (QT) is key to understanding the behavior of neutron stars, thereby using them to probe the properties of nuclear matter in neutron-rich environments – a core aspect of the DoE mission. For example, turbulence from the interacting superfluid vortices in the neutron star crust is expected to explain puzzling phenomena such as pulsar glitches – sudden rapid increases in the rotation rate of neutron stars despite continuous loss of energy and angular momentum – thereby connecting astrophysical observations with the superfluid dynamics. Enabling these observations to constrain nuclear physics is one of the most demanding multi-scale problems in physics, connecting femtoscale nuclear physics with kilometer-scale astrophysics. This project simulate quantum turbulence in strongly interacting fermionic superfluids, allowing us to characterize for the first time how kinetic energy is distributed over various length scales – a key characterization of quantum turbulence. We will compare our results with similar characterizations for bosonic superfluids, highlighting the differences between fermionic and bosonic superfluids. This characterization will provide a rigorous underpinning of the vortex filament model and viscous hydrodynamic theories needed to model macroscopic volumes of neutron stars.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Energetics of Collisionless Plasmas in the Laboratory and Space

Principal Investigator: Will Fox, Princeton Plasma Physics Laboratory

Co-Investigators: K. Germaschewski, Unversity of New Hampshire

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
62,000 node hours

Research Summary

Understanding the processes which convert energy between different forms — magnetic energy, flow energy, thermal energy, and accelerated particle populations — is a key unifying question of plasma astrophysics. The key processes — magnetic field generation by Weibel instability and the Biermann process; magnetic field destruction by magnetic reconnection; and flow thermalization by magnetized shocks — can potentially explain some of the most important questions in astrophysics, including acceleration of high energy particles such as cosmic rays, which are the highest-energy particles observed in the universe, millions of times more energetic than can be produced at earth-bound particles accelerators. Magnetic reconnection is ubiquitous in fusion, space and astrophysical plasmas, playing a central role in liberating stored magnetic energy in phenomena as diverse as sawtooth crashes in fusion plasmas, magnetospheric substorms, and solar flares. The Weibel instability is of great interest as one of the few known processes that generates magnetic field de novo in laboratory and astrophysical plasmas, enabling formation of collisionless shocks driven by astrophysical explosions such as supernova remnants and gamma ray bursts. Both problems are grand-challenge, multi-scale problems, where macroscopic flows and fields are coupled to microscale current sheets (in the reconnection case) and shock transition layers (for collisionless shocks). Both processes (reconnection and shocks) have been proposed to accelerate cosmic rays.

The proposed ALCC project will use Summit at OLCF for simulations with the plasma particle-in-cell code PSC, which allows fully kinetic simulations with a 1-1 matching of plasma parameters between simulation and laboratory experiments, allowing exploration of the physics under laboratory conditions, generating experimental predictions, and allowing tests of the fundamental understanding against the ground truth of experiments. Results will be compared with ongoing experiments on magnetic reconnection, Weibel instability, and collisionless shocks in laser-produced plasmas conducted at the Omega-EP facility at the University of Rochester and the National Ignition Facility at LLNL.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Metastability in Driven Dynamical Systems for Next-Gen Microelectronics Applications

Principal Investigator: Panchapakesan Ganesh, Oak Ridge National Laboratory

Co-Investigators: Adrianus van Duin, Penn State University ,
Dundar Yilma, Penn State University,
Nouamane Laanait, Oak Ridge National Laboratory,
Rama Vasudevan, Oak Ridge National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
500,000 node hours

Research Summary

Advances in microelectronics, especially low-power electronics and novel forms of computing, require fundamental breakthroughs that limit our ability to predict how microelectronics behave under 'high' time-varying fields. Recent proposals for analog devices using new materials are attractive for enabling brain-like neuromorphic computing. Similarly, proposals for novel transistors using conventional ferroelectrics boast of improving their energy efficiency limits significantly. Understanding how to stabilize ferroelectrics in the negative-capacitance regime has been identified as a key-challenge to enable "New Electronic Materials and Phenomena for Information and Energy Transfer" in the recent DOE-BES Basic Research Needs for Microelectronics document. Brain-inspired neuromorphic computing – which may use memristive components – has been identified as a complimentary architecture enabling a key principal research direction for "Revolutionizing memory and data storage".

Fundamental challenges remain – while metastability is required to obtain memory-effects in memristive materials it is not clear how they form under high-fields, what their dynamical response is at fields/temperatures and how we can control them. Similarly, we do not know how ferroelectrics with intrinsic (or extrinsic) defects switch as well as their role in stabilizing polarization in the negative capacitance state and achieving large intrinsic dielectric tunability. Thus, understanding how metastability is encoded and accessed in defective materials can enable us to address these challenges and redefine computing by leveraging unexploited physical phenomena, a key priority research direction indicated in the DOE-BES report mentioned above.

This project will address these challenges in ferroelectrics using a new approach that more accurately simulates dynamical responses of a defective ferroelectrics under realistic fields and temperatures and can scale to several millions-of-atoms and validate predictions with existing experiments. The project will also apply state-of-the-art machine-learning methods to accelerating the molecular-dynamics simulations and for obtaining insights about the dynamics.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Large Scale Numerical Simulations of Polymer Nanocomposites

Principal Investigator: Gary Grest, Sandia National Laboratory

Co-Investigators: Shengfeng Cheng, Virginia Polytechnic Institute and State University
Ting Ge, University of South Carolina
Sanat K. Kumar, Columbia University
Dvora Perahia, Clemson University
Michael Rubinstein, Duke University

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
325,000 node hours

National Energy Research Scientific Computing Center (NERSC)
150,000 node hours

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. Our 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. Specifically, we seek to resolve the factors that control the assembly of multiple nanoparticles in bulk materials and in thin films. As producing polymer nanocomposites with well-dispersed fillers is a major hurdle for making new materials, we will concentrate our studies on identifying the parameters that control nanoparticle dispersion. One approach we will explore for dispersing nanoparticles in a polymer matrix is to separately optimize the enthalpic and entropic components by end-grafting a mixture of short and long chains to the nanoparticle. The short chains are to screen the enthalpic interaction between nanoparticles while the long chains mix with the polymeric matrix, producing enhanced mechanical and thermal stability. As many polymer films are made by first dissolving the nanoparticles and polymer in a solvent and then evaporating the solvent, we model the effect of solvent evaporation rate on the dry polymer film. Rapid solvent evaporation can lead to long-lived metastable states in which the nanoparticles are trapped in the polymer film, providing a means to disperse nanoparticles when in equilibrium they would aggregate. Rapid drying can also be utilized to create controllable stratified distributions of nanoparticles in a polymer matrix. We finally determine the rheological response and mechanical properties of the resulting polymer nanocomposites and study molecular transport through polymer nanocomposite membranes for gas separation.

Motivated by the numerous potential applications of polymer nanocomposites with unique new properties, we will use large-scale molecular dynamics simulations to define the interaction of nanoparticles and control their miscibility in polymer melts and their self-assembly that will serve as building blocks for new materials and device.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Nucleon Matrix Elements: Probes of New Physics

Principal Investigator: Rajan Gupta, Los Alamos National Laboratory

Co-Investigators: T. Bhattacharya Los Alamos National Laboratory,
V. Cirigliano, Los Alamos National Laboratory
B. Yoon, Los Alamos National Laboratory,
B. Joo, Jefferson Laboratory,
H-W Lin, Michigan State University

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

National Energy Research Scientific Computing Center (NERSC)
670,000 node hours

Research Summary

Large scale simulations of lattice quantum chromodynamics (QCD) allow us to calculate matrix element of operators (interactions) composed of quarks and gluons to quantify a number of properties of protons and neutrons at the hadronic scale of a few GeV. These, combined with precision experiments, allow us to probe new interactions and symmetries at the TeV scale. In this proposal, we focus on the axial vector form factors of the nucleon that are needed to calculate the cross-section for neutrino-nucleon scattering. Reaching a precision of 2% in the cross-section over a range of energies is needed to discover charge- conjugation-parity (CP) symmetry violation in the neutrino sector, the goal of the Deep Underground Neutrino Experiment (DUNE) experiment at Fermilab We will use large scale simulations of the fundamental theory of strong interactions, QCD, discretized on a 4-dimensional Euclidean lattice for the calculations. Over the last year we have resolved a major systematic that afflicted all previous lattice calculations of the axial form factors. We are now in a position to perform a full scale calculation that will provide results with reliable estimates of statistical and all systematic errors.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Artificial Intelligence Directed Adaptive Multiscale Simulations to Model RAS-RAF Cancer Initiation Pathway

Principal Investigator: Harsh Bhatia, Lawrence Livermore National Labortatory

Co-Investigators: Helgi I. Ingólfsson, Lawrence Livermore National Laboratory
Arvind Ramanathan, Argonne National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
600,000 node hours

Research Summary

Whereas computational models can define the functional dynamics of complex systems in exceptional detail, phenomena of interest can typically be simulated either with high-resolution (microscopic) detail or with a coarser representation over large (macroscopic) length- and time-scales. Multiscale modeling and simulations, which aim to bridge this gap, are often key to reliable exploration of complex physical, chemical, and biological phenomena. However, high-fidelity simulations already occupy over 45-60% of available computer time on existing supercomputing resources. Capturing coupled processes within multiscale simulations for systems of increasing size and complexity, especially as multiscale approaches must explore millions of configurations, quickly exceeds the limits of contemporary computational capabilities. Emerging Exascale architectures pose additional computational challenges for multiscale simulations. Hence, incremental approaches to multiscale simulation software will not be sufficient for optimizing the overall throughput of large-scale multiscale simulations.

The project will validate multiscale simulations that are guided by machine learning techniques to significantly improve both the length- and time-scales accessed by these simulations, and make reliable decisions for time-sensitive experiments/applications. As part of an ongoing DOE-NCI collaboration, the project team has developed *Multiscale Machine-learned Modeling Infrastructure* (*MuMMI*), which represents a new paradigm of multiscale simulations and enables exploring large length- and time-scales (microns and seconds, respectively) using *macro-level models*, while simultaneously maintaining molecular- and atomistic-scale details using a novel ML-based sampling framework.

Specifically, the project will study a complex biological phenomenon – the cancer initiation pathway mediated by the RAS and RAF oncogenes. RAS and RAF are important links in the cell's signaling system and nearly a third of all cancers diagnosed in the U.S. are driven by mutations in RAS genes and their protein products. Aberrant RAS behavior accounts for a particularly high percentage of pancreatic (~95%), colorectal (~45%), and lung (~35%) cancers. Previous work focused on exploring the role of RAS in the pathway as well as some initial studies on RAF, this project will extend MuMMI to decipher more complex aspects of the initial triggering of RAS-RAF signaling near the membrane using *three* resolutions (macro, coarse-grained, and atomistic) of simulations delivering insights into relevant behavior.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Gyrokinetic Simulations of Multi-Scale Plasma Turbulence in Tokamaks

Principal Investigator: David Hatch, University of Texas at Austin

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
69,000 node hours

National Energy Research Scientific Computing Center (NERSC)
30,000 node hours

Research Summary

First-principles-based whole device modeling (WDM) of fusion devices is one of the great frontiers of computational plasma physics. Ultimately, success will enable the confident exploration of new ITER scenarios and new reactor concepts *in silico*, at greatly reduced cost and over a much wider range of possibilities. The challenges associated with connecting simulations of physical processes occurring at vastly different time and space scales to one another are immense and will require significant computational resources. In this project we are pursuing multi-scale simulations of turbulence in the crucial edge transport barriers of tokamaks using the gyrokinetic code GENE. This challenge must be addressed in order to achieve first principles WDM capability.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Benchmarking Many-Body Perturbation Theory

Principal Investigator: Olle Heinonen, Argonne National Laboratory

Co-Investigators: Anouar Benali, Argonne National Laboratory,
Marco Govoni, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

Accurate calculations of excitation energies in molecular systems are paramount for a wide spectrum of important energy-related applications, such as catalysis, photo-absorption, and synthesis as well as for areas such as quantum materials, in particular those with strong correlations for which many standard methods do not work well. The most accurate quantum-chemical computational methods suffer from poor scaling and rapidly become unusable as the size of molecules grow. Many-body perturbation theory (MBPT) yields neutral and charged excitations of molecules and materials by solving the Dyson and Bethe Salpeter equations in a perturbative manner, starting from the output of a Density Functional Theory (DFT) calculation. While MBPT methods scale better than quantum chemical methods, they have traditionally been rather expensive, and the accuracy of the results are sometimes difficult to assess and also tend to depend on the starting point of the calculations. Quantum Monte Carlo methods, on the other hand, are in principle exact but in practice suffer from the fixed-node approximation, and until recently, systematic attempts to improve on this approximation have been difficult to implement.

In this project we will use newly implemented multi-reference (MR) quantum Monte Carlo (QMC) methods to provide reference data for parallelized MBPT calculations of several molecular sets and explore approaches to improve their accuracy. The QMC MR method for molecular systems is based on selected Configuration Interaction . This method, known as Configuration Interaction using a Perturbative Selection made Iteratively (CIPSI), is used to systematically construct a multi-determinantal trial wavefunction that can be used in QMC, and was able to efficiently and accurately describe strongly correlated ground states and any exited state for a large class of molecules . We will first determine the optimal conditions for MBPT and explore avenues to systematic improvements on GW and BSE, as well as to DFT methods. This work will utilize the DOE-supported codes Qbox/West and QMCPACK.

Title: Plasma-Based Acceleration of Protons & Elucidation of Mechanisms

Principal Investigator: Axel Huebl, Lawrence Berkeley National Laboratory

Co-Investigators: Jean-Luc Vay, Lawrence Berkeley National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
108,000 node hours

Research Summary

Based on the Nobel-prize winning technology (2018) proposed by Strickland & Mourou, ultra-high intensity, ultra-short, petawatt-class (PW) laser pulses became recently available to the scientific community and are being actively used for scientific discoveries. One of the pressing fields of research is laser-driven ion acceleration, which strives for compact sources of ion and proton beams for critical societal challenges such as the democratization of hadron therapy, basic high-energy-density physics research and as potential sources for compact, ultrafast imaging of dense materials.

Experimental studies on first PW-class laser facilities have been ongoing for several years, yet controlling the beam stability and charge while at the same time achieving the highest maximum energy remains an unsolved challenge.

In this project, we will improve the modeling capabilities of laser-ion accelerators in several ways. First, high resolution simulations will be used to adequately describe the laser-target interaction and geometric target expansion on the femtosecond time scale. This will present a significant improvement since simulations with reduced dimensions and resolution are often unable to adequately predict the maximum particle energy and acceleration dynamics for petawatt-class experiments. Second, WarpX' unique mesh refinement technique, implemented in a fully electromagnetic particle-in-cell loop will be used for the first time to deliver higher spatio-temporal resolution for the target while avoiding over-resolution of areas that only contain lower-density plasma and long-standing fields. We will use these capabilities to explore novel target systems for laser-ion acceleration in close collaboration with experimental teams at LBNL and collaborators and to model the sensitivity of underlying acceleration mechanisms to the conditions present at leading PW-class laser facilities.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Interpretable Machine Learning Force Fields for Accurate Chemical Reactive Dynamics

Principal Investigator: Olexandr Isayev, Carnegie Mellon University

Co-Investigators: Adrian Roitberg, University of Florida,
Alvaro Vazquez-Mayagoitia, Argonne National Laboratory,
Dmitry Lyakh, Oak Ridge National Laboratory,
Dmytro Bykov, Oak Ridge National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
350,000 node hours

Research Summary

Efficient combustion of low-carbon fuels have been identified by DOE as one of the areas where predictive simulations can have a large impact. These simulations require knowledge of high-accuracy chemical kinetic reaction mechanisms that capture the complex chemistry of pyrolysis, hydrocarbon growth and oxidation dynamics. Traditional methods to study these mechanisms rely on empirical knowledge of elementary reaction types, rate measurements for some of these reactions, and educated guesswork for the rates of other reactions. Recent studies also include a small number of reaction rates calculated theoretically. Yet, with this approach, new kinetic reaction mechanisms can take many years to develop. Things get even more complicated on the simulation side when chemical reactions involve low- lying excited electronic states photo-activated by light, for which reliable force fields are hardly available. The ability to provide fast and accurate quantitative description of a broad class of such photocatalytic gas-phase reactions would have an immediate impact on the research geared towards photo-activated CO2 reduction, water splitting, the oxidation of volatile organic compounds, the degradation of NOx, and the synthesis of ammonia.

The overall goal of this project is to train and deploy an interpretable neural network force field capable of predicting reaction energetics and rates for chemical reactions with high accuracy, but with a very low computational cost, with proof-of-principle applications in simulations of combustion processes and gas-phase photo-dynamics. This will be accomplished by training a deep neural network model on a set of atomic configurations representing typical reaction pathways and transition states between chemical reaction intermediates. The resulting quantum-mechanically informed force field potential for ground and excited electronic states implemented in a neural network code will be integrated as a module in Python- based Atomic Simulation Environment, LAMMPS, AMBER, and OpenMM software packages, and delivered to a broader community via GitHub.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Global Climatype Clustering: Precision Agriculture for Bioenergy

Principal Investigator: Daniel Jacobson, Oak Ridge National Laboratory

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
400,00 node hours

Research Summary

The human population is predicted to reach 9 billion by 2050, which will require a significant expansion of biofuel products to address sustainable energy needs as well as a 70% increase in food production (and a doubling in developing countries). These challenges necessitate detailed and accurate knowledge of environmental conditions on a global scale to rapidly establish crops in geographic regions that will maximize production and minimize costs. Furthermore, as productive lands become abandoned due to changing climate conditions, there is a need to match plants to appropriate environments or engineer new plant varieties that are hardy in less favorable conditions. We now have the ability to design plant genotypes (cultivars) that are optimized for energy production, are stress resistant, and can be grown in targeted locations where they are likely to thrive. This will allow us to develop highly productive plant cultivars that can take advantage of land not currently used for agriculture in order to help meet the growing sustainable energy needs of an expanding human population in the context of a changing climate. Of critical importance to these efforts is the method of determining high resolution climate zones for which plants can be engineered.

This project will analyze the daily climate patterns across many environmental variables for each square kilometer of dry land across the planet to improve our understanding of climate zones and fine-scale geographic conditions. Additional analyses will build on those results to make accurate and unbiased assessments of environmentally correlated regions that can be used to address the problems of energy and food security. The application of high performance computing and explainable-Artificial-Intelligence to these problems will make it possible to engineer crops that are more resource efficient, stress resistant, and better able to thrive in modified lands.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Electronic Structure and Excited States Dynamics of Quantum Materials

Principal Investigator: Jacek Jakowski, Oak Ridge National Laboratory

Co-Investigators: Jerry Bernholc, North Carolina State University,
Mina Yoon, Oak Ridge National Laboratory,
David Lingerfelt, Oak Ridge National Laboratoroy,
Panchakepasan Ganesh, Oak Ridge National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
180,000 node hours

Research Summary

This proposal aims at simulations of quantum materials and systems for quantum information processing applications. We will utilize DFT and time-dependent DFT methods to model the electronic properties, transformations and excited state dynamics in 2D materials. We propose to investigate 2D quantum systems that will be used in future computers and circuits: (1) single photon emitters, necessary to communicate between various parts of quantum computers, (2) quantum dots that can be used to design high-temperature qubits, and (3) transduction between topologically-protected quantum-states that could be potentially used as qubits for quantum-computations. We will focus on electronic excitations in a topologically protected 'realistic' interfacial system, and study transient topologies when the system is excited using an electron beam or optical light. Our theoretical approaches range from DFT and hybrid-DFT methods to time-domain simulations (based on RT-TDDFT) of excited electrons. Our computational design of topological quantum dots is based on the experimental capabilities at ORNL. Our computational modeling will guide the experimental effort of engineering defects and dopants in 2D materials to convert them into new types of topological quantum dots. The formation of defects and dopants in 2D materials and their time-evolution dynamics will be investigated using ab initio molecular dynamics. We will then investigate the defect/dopant response to optical, electronic, and thermal excitations and identify the most desirable types of defects and dopants that could serve as quantum qubits.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Study of a Disrupting Plasma in ITER

Principal Investigator: Stephen Jardin, Princeton Plasma Physics Laboratory

Co-Investigators:

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
30,000 node hours

Research Summary

The ITER device being constructed in Cadarache, France is a monumental step towards the realization of fusion power. The $40+ B experiment, financed by seven international governments including the U.S., will pave the way for a demonstration fusion power plant to be built on the same scale. Success in this endeavor will be a turning point in the quest for a sustainable, carbon-free, safe and nuclear-proliferation- free source of energy for the planet.

ITER is a type of doughnut-shaped fusion device known as a tokamak. The fully ionized gas (called plasma) within ITER will be heated 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 super-conducting electromagnets. Large electrical currents flowing in the tokamak plasma itself produce additional magnetic fields that are essential.

We are collaborating with other researchers in Italy to predict the forces on the ITER vacuum vessel and other metallic structures in the event of a "worst case" VDE in which control is lost of a tokamak plasma carrying the full design value of 15 million Amperes of electrical current (15 MA). The Italian group, through consortium CREATE, has developed a detailed engineering model of the ITER vacuum vessel and other structures using the electro-mechanical code they developed called CARRIDI. We have recently developed techniques to couple the M3D-C1 code describing the tokamak plasma with the CARRIDI code describing the response of the structure. This proposal is to apply these codes to the present ITER design in order to quantitatively predict the consequences of the discharge becoming unstable. This demanding calculation represents a capability unique in the world.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Stochastic A Priori Dynamics for Complex Reactive Chemical Environments

Principal Investigator: Ahren Jasper, Argonne National Laboratory

Co-Investigators: Daniel Moberg, Argonne National Laboratory,
Christopher Knight, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

The outcome of a gas phase chemical reaction results from the competition of a variety of underlying microscopic dynamical processes, including bond breaking and forming, energy transfer and redistribution, and quantum mechanical events like tunneling and electronic transitions. High performance computing and methodological advances in electronic structure theory and semiclassical dynamics have led to dramatic increases in the fidelity of a priori predictions of isolated chemical events. Significant challenges remain, however, in the a priori characterization of more complex reactive chemical environments, such as flames and chemical reactors, that are central to many energy technologies.

Here we propose to apply a theoretical framework for predicting the chemistry of complex systems, in both the gas phase and extended phases, that is readily parallelizable and scalable and that leverages high performance computing. The approach combines high-accuracy theoretical methods for elementary dynamics employing ab initio potential energy surfaces and including semiclassical treatments for nonadiabatic transitions, tunneling, and zero-point energy maintenance. Competition between these events is modeled stochastically in order to treat networks of reactions and access long timescales. The resulting stochastic a priori dynamics approach is designed to enable predictive discovery in systems with use- inspired complexities, and it is distinct from phenomenological approaches being pursued elsewhere.

We will consider two related applications to study the competition of collisional stabilization and reactivity and to demonstrate the utility of the approach. In the first set of applications, nonequilibrium and nonthermal events in many body gas phase systems will be characterized at atmospheric and combustion conditions where the usual assumption of abundant thermalizing collisions between reactive events breaks down. In the second set of applications, lower temperatures will be considered where nuclear quantum effects are important, and we will study the reactivity of transient dimers, as in the so-called “chaperone effect” that emerges at high pressures, and more generally the reactivity of small van der Waals clusters.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Nucleon Axial Charge with All-Staggered Lattice QCD

Principal Investigator: Andreas Kronfeld, Fermi National Accelerator Laboratory

Co-Investigators: Steven Gottlieb,Indiana University,
Aaron Meyer,Brookhaven National Laboratory,
James Simone, Fermi National Accelerator Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
200,000 node hours

National Energy Research Scientific Computing Center (NERSC)
870,000 node hours

Research Summary

We propose to take the next step in demonstrating that staggered valence quarks are a viable strategy in lattice quantum chromodynamics (QCD) for nucleon physics. Recently, our methodology has been applied to obtain the most precise calculation of the nucleon mass to date [arXiv:1911.12256]. Here we propose to compute the nucleon axial charge, a hadronic matrix element entering the neutron decay rate and, simultaneously, the normalization of the nucleon axial form factor. The latter is a key nucleonic ingredient in estimating the neutrino-nucleus cross sections and, thus, an underpinning of the Fermilab neutrino program (culminating in LBNF/DUNE). The axial charge is, thus, a crucial stepping stone en route to the form factor's kinematic dependence.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Characterizing Coastal Low-Level Jets and their Impact on Offshore Wind Farms

Principal Investigator: Jing Li, GE Research

Co-Investigators: Umesh Paliath, GE Research

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
190,000 node hours

Research Summary

Wind energy is playing an increasingly greater role in this nation's energy future which brings profound impacts: meeting the growing energy need by providing cost-competitive power, strengthening energy security by diversifying the supply, and curbing global climate change by reducing greenhouse gas emissions. DOE envisions wind to supply 20% of U.S. energy by 2030 in which the offshore wind sector is an integral part. However, one impediment to the growth of U.S. offshore wind energy is a lack of thorough understanding of offshore wind conditions and the corresponding turbine behaviors. One prevalent yet poorly understood wind phenomenon is the coastal low-level jets (LLJ). As opposed to the commonly observed log-law wind profiles in the atmospheric boundary layer, LLJ are anomalous wind events associated with a nonmonotonic profile. Currently, observational data is scarce and usually not at the spatiotemporal accuracy required to fully characterize LLJ. High-fidelity simulations may be employed to bridge the gap, however LLJ are very challenging to predict and require detailed multiscale simulations of atmospheric turbulence which require enormous computational capacity.

This project will provide, for the first time, high-resolution description of the turbulent atmospheric flow, wind farm flow, and wind turbine performance under U.S. North Atlantic coastal LLJ wind condition. In achieving these goals, this project will advance our understanding of offshore wind conditions and improve the safe and efficient operation of offshore wind farms, increasing competitiveness of U.S. offshore wind industry and contributing to DOE's mission of ensuring U.S. energy security.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Unveiling the 3D Structure of Nucleons with Machine Learning and Lattice QCD

Principal Investigator: Hueywen Lin, Michigan State University

Co-Investigators: Simonetta Liuti, University of Virginia

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
660,000 node hours

Research Summary

Nucleons (that is, protons and neutrons) are the building blocks of all ordinary matter, and the study of nucleon structure is a critical part of frontier research to unveil the mysteries of the universe and our existence. Gluons and quarks are the underlying degrees of freedom that explain the properties of nucleons, and fully understanding how they contribute to the properties of nucleons (such as mass or spin structure) helps to decode the last part of the Standard Model that rules our physical world. After more than half a century of experiments, there are still many unknowns concerning the theory quantum chromodynamics (QCD), a branch of the Standard Model, describing how gluons strongly interact with themselves and with quarks, binding both nucleons and nuclei. Due to their confinement within these bound states, we cannot single out individual particles to study, and the predicted state that is made up of gluons only has yet to be experimentally observed. To date, we still know little about the nucleon's three-dimensional structure, which is characterized by functions such as the generalized parton distributions (GPDs). The GPDs can be viewed as a hybrid of parton distributions, form factors and distribution amplitudes. They play an important role in providing a three-dimensional spatial picture of the nucleon and in revealing the spin structure of the nucleon. Experimentally, GPDs can be accessed in exclusive processes such as deeply virtual Compton scattering or meson production, an important DOE mission which is ongoing at Jefferson Lab and the future Electron-Ion Collider (EIC) in the US. Using the theoretical tool lattice QCD (LQCD) to provide additional inputs and leveraging machine learning to combine experimental inputs, we will produce the best three-dimensional images of nucleon.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Large eddy and convection-permitting simulations of aerosol-cloud interactions

Principal Investigator: Po-Lun Ma, Pacific Northwest National Laboratory

Co-Investigators: Colleen Kaul, Pacific Northwest National Laboratory,
Kyle Pressel, Pacific Northwest National Laboratory

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
300,000 node hours

Research Summary

Accurate simulation of aerosol-cloud interactions remains a major challenge for Earth system models. Significant uncertainties are attributed to coarse resolution and limitations in process representations. In contrast to traditional coarse-resolution models, the global convection-permitting resolution planned for the Energy Exascale Earth System Model (E3SM) version 4 provides a path toward accurate estimation of aerosol effects. However, parameterizations still need to be redesigned to better represent aerosol and aerosol-cloud interactions processes at convection-permitting resolution and to perform efficiently on DOE's leadership Computing Facilitites.

This project will perform limited-area large-eddy simulations (LES) and convection-permitting simulations to develop new parameterizations and assess their impacts on the Earth system. These simulations will be used as part of DOE's multi-year Earth System Model Development (ESMD) project, Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES), which integrates expertise in atmospheric and computational sciences to increase confidence in, and understanding of, the role of aerosols and aerosol-cloud interactions in the evolution of the Earth system using new modeling techniques that are scientifically robust and computationally efficient for global convection-permitting simulations.

An LES model will be run over a wide range of aerosol and cloud regimes to construct a large ensemble to provide sufficient data for the reformulation of precipitation process and droplet nucleation and for building emulators using novel machine learning algorithms (e.g., convolutional neural network). A nonhydrostatic version of the E3SM with a regionally refined mesh (RRM) will be used for four regions (Eastern North Atlantic, Central U.S., Northeast Pacific, and Southern Ocean) to assess the impacts of new parameterizations on aerosols and aerosol-cloud interactions in various conditions. Computational cost for individual processes will be analyzed for performance optimization.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Many-Body Perturbaiton Theory Meets Machine Learning to Dicover Materials for Organic Photovoltaics

Principal Investigator: Noa Marom, Carnegie Mellon University,

Co-Investigators: Volker Blum, Duke University,
Patrick Rinke, Aalto University, Finland

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

Organic solar cells have several appealing advantages: they are made of earth-abundant elements; they can be manufactured cheaply over large areas via solution deposition and printing techniques; they may be deposited on oddly shaped and/or flexible surfaces; they are lightweight; and most importantly, their electronic properties may be tuned over a broad and almost continuous range through chemical and structural modification. These properties make them attractive, particularly for low- cost, large area applications as well as for wearable and disposable devices. However, the present efficiency of organic photovoltaics leaves much to be desired.

The proposed research may accelerate the discovery and deployment of new materials for better organic solar cells by combining quantum mechanical simulations with machine learning. The materials properties of interest for solar cells are derived from electronic excitations. This calls for theoretical treatment beyond ground-state density functional theory (DFT). This will be achieved by Green's function based many-body perturbation theory (MBPT), within the GW approximation and Bethe-Salpeter equation (BSE). The relatively high computational cost of GW+BSE simulations makes them impractical for large- scale high-throughput materials screening. Therefore, we will develop machine learned models that will be trained on DFT and MBPT data and, once sufficiently predictive, used for materials screening. The Artificial Intelligence for Spectroscopy (ARTIST) library will be used to predict properties from molecular structural information. The sure independence screening with sparsifying operators (SISSO) feature selection algorithm will be used to identify descriptors that are fast to evaluate and predictive of MBPT data. To accelerate data acquisition, we will speed-up and improve the scaling of the GW+BSE implementation in FHI-aims. This will be achieved by using a local resolution of identity (RI) approach and improved parallelization of the BSE kernel matrix setup.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Influence of Antarctic and Greenland continental shelf circulation on high-latitude oceans in E3SM

Principal Investigator: Julie L. McClean, Scripps Institution of Oceanography, UC San Diego

Co-Investigators: Sarah T. Gille, Scripps Institution of Oceanography, UC San Diego
Mathew E. Maltrud, Los Alamos National Laboratory
Detelina P. Ivanova, Scripps Institution of Oceanography, UC San Diego

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
200,000 node hours

Research Summary

The Greenland and Antarctic Ice Sheets have undergone accelerated mass loss over the past decades. Basal melt rates (ocean melting) within Antarctic ice shelf cavities have surpassed those by iceberg calving along much of the Antarctic shelf. Mass loss at Greenland Ice Sheet margins due to ocean interactions is currently estimated to contribute about 50% to the total Greenland Ice Sheet loss; this total amounts to about one quarter of observed global sea level rise. Antarctic Ice Sheet mass loss is roughly half that of the total Greenland loss. In addition to global sea level rise, the increasing amounts of freshwater entering the ocean produce changes in ocean stratification and sea-ice distributions, which in turn, impact heat and moisture exchanges with the atmosphere.

Reliable projections of future Earth System conditions are needed for policy makers. The greatest source of uncertainty in current sea level rise projections to date is the contribution from land-ice melt. Explicit simulation of mesoscale ocean eddies and processes has been found necessary to realistically simulate many physical processes important to climate. In this context, they are important in the delivery of anomalously warm ocean water across the continental shelf to the land-ice/ocean interface. An interim step therefore, is to include a representation of the freshwater fluxes arising from both Greenland and Antarctic Ice Sheet melt in global high-resolution ocean/sea-ice models.

This project will model the processes responsible for transporting heat across the Antarctic and Greenland continental shelves to the land-ice/ocean interfaces and the impacts of freshwater input caused by land-ice melt. The allocation will enable the team to complete the first-generation mesoscale eddy-resolving global ocean simulation with the capability to represent a broad spectrum of physical processes in the study regions that to date have not been simulated in a global model. Comparisons between it and lower-resolution counterpart models will be used to identify regions where realistic simulation of land-ice/ocean/sea-ice interactions require enhanced resolution.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Toward Full Core Multiphysics High Fidelity Calculations

Principal Investigator: Elia Merzari, Pennsylvania State University

Co-Investigators: Jun Fang, Argonne National Laboratory
Dillon Shaver, Argonne National Laboratory,
Derek Gaston, Idaho National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
150,000 node hours

Research Summary

Nuclear energy power promises to become a reliable, carbon-free resource capable of meeting our nation's and the world's energy needs. Amid an increase in cost of traditional nuclear reactor designs, in recent years, advanced reactor concepts have emerged as an attractive solution capable of significantly increasing inherent safety while reducing cost. Modeling and simulation plays a vital role in the deployment of such advanced systems. As a consequence, both DOE-NE, through the Nuclear Energy Modeling and Simulation program, and DOE-SC/ASCR have invested in the modeling of advanced reactors.

The proposed work will generate high-fidelity datasets for advanced reactor designs, including integral PWR SMRs. High-fidelity multiphysics simulations will be performed using Nek5000 and BISON, state- of-the-art codes for the three-dimensional modeling at high fidelity of fluid flow, heat transfer and fuel performance. In particular, we will perform wall-resolved large eddy simulation (LES) of the flow in portions of the reactor core using the spectral element code Nek5000.

Essential for such challenging simulations is access to leadership-class computational resources and in particular, Summit. Nek5000 has been recently ported to GPUs with excellent performance (NekRS). The simulations will use geometric information available in the open literature and will generate vast datasets (e.g., first- and second-order statistics, budgets, correlations) that can be used to inform lower-fidelity models (porous media, systems codes and subchannel codes).

This activity is funded as a high priority activity in the newly formed Center of Excellence for Thermal- Fluids Applications in Nuclear Energy funded under the Nuclear Energy Modeling and Simulation program.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Portable Performance on Exascale Hybrid Architectures

Principal Investigator: Bronson Messer, Oak Ridge National Laboratory

Co-Investigators: Jack Deslippe, Lawrence Berkeley National Laboratory,
Tim Williams, Argonne National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
130,000 node hours

Research Summary

Scalability and node-level, GPU-based performance are increasingly important to effetive utilization of HPC resources. All three of DOE's open science HPC facilities have application readiness programs to enable mission critical applications to be ready to effectively utilize new systems on day one of operations. This project will provide large-scale development resources to all three application readiness programs currently underway at NERSC, ALCF, and OLCF – all three are deploying GPU enabled upgrades in the 2021-2022 timeframe. Summit is the only available resource that can provide both hybrid node architecture and ample scale for development of many of these codes. The multiple projects span many scientific areas, numerical approaches, and combinations of simulation, data, and learning. All of the application codes involved have already demonstrated parallel performance at the level of INCITE-readiness on present-day systems. Much of the work to be done on these applications is centered on single-node parallelism. However, constant monitoring of scalability will also be necessary to ensure the codes will be able to meet the scientific objectives of each of the subprojects. Projects involving data intensive and Machine Learning/Directed Learning approaches will also look at scalability and component integration (in addition to single-node parallelism).

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: High temperature material properties from first principles

Principal Investigator: Mark Messner, Argonne National Laboratory

Co-Investigators: Sam Sham, Argonne National Laboratory,
Roberto Pasianot, National Atomic Energy Commission, Argentina,
Hugo Mosca, National Atomic Energy Commission, Argentina,
Sebastián Jaroszewicz, National Atomic Energy Commission, Argentina

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
200,000 node hours

Research Summary

Traditional structural engineering design considers only time-independent failure modes: either a structure will immediately fail under some combination of loads or it will not. In contrast, for high temperature structural components failure is governed by time-dependent creep. Therefore, to design safe and effective structural components for next-generation high temperature nuclear reactors, concentrating solar power systems, supercritical fossil fuel plants, and petro-chemical processing facilities engineers need to know how a material will behave under very long periods of load at high temperatures. This information is often not available because of the very long time required to complete the necessary experiments.

Ideally, we could generate the required time-dependent material properties from first-principles simulations upscaled to engineering properties using multiscale, physics-based models. This would reduce or avoid lengthy tests and decrease the time between the discovery of a new material and the point it actually enters service. However, there are two key challenges in advancing models of high temperature structural deformation and damage down to the atomistic length scale: 1) Time scale -- MD simulations typically span microseconds at best, creep deformation occurs over a period of years; and 2) Modeling sufficient defects -- creep deformation depends on defects in the metal's crystal lattice (dislocations, vacancies, and voids), not the bulk lattice properties. Relevant MD calculations would need to contain enough atoms to represent a statistically meaningful quantity of defects.

To address the first issue we are proposing to use a novel multiscale method based on homogenizing the rate of state variables, rather than the variables themselves, interpolating sparse MD data with machine learning techniques, and assuming steady state behavior to extrapolate in time. We propose to address the second issue with large-scale use of HPC. Recent results published in Nature (Zepeda-Ruiz et al., 2017) demonstrate the MD calculations with size from 15M to 300M atoms are both feasible with current HPC resources and provide information that is directly-relevant to crystal plasticity modeling.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Probing QCD crossover with hyper-skewness and hyper-kurtosis

Principal Investigator: Swagato Mukherjee, Brookhaven National Laboratory

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

Under extreme conditions of high temperatures and/or densities hadrons cease to exist— quarks and gluons are liberated from the hadrons to form a new state of matter, known as the quark qluon plasma (QGP). A central goal of the experimental programs at the Relativistic Heavy-Ion Collider (RHIC) of the Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN, Switzerland is the exploration of the phases of strong-interaction QCD matter. At LHC and higher RHIC energies the transition from the QGP to hadrons is expected to occur through a smooth crossover. Hyper-skewness and hyper-kurtosis, i.e., the fifth and sixth order cumulants, of baryon, charge and strangeness fluctuations are sensitive probes for detecting the crossover nature of the hadron to QGP transition. Experimental measurements of hyper-skewness and hyper-kurtosis are underway as part of the RHIC Beam Energy Scan (BES) program, and are a high-priority for the soon-to-come high-luminosity LHC upgrade.

The cumulants of conserved charge fluctuations also can be computed starting from the fundamental theory of strong interaction— quantum chromodynamics (QCD)— using large-scale numerical calculations of the lattice-regularized version of the theory. Using state-of-the-art lattice QCD calculations we will provide the QCD-baseline for the hyper-skewness and hyper-kurtosis of conserved charge fluctuations, which can be confronted directly with experimental findings at RHIC BES and LHC. Furthermore, these QCD calculations will enable determinations of the QCD-baseline for skewness and kurtosis of conserved charges at larger values of baryon densities, which are crucial for detecting the QCD critical point. These computations also will provide other QCD-inputs needed to decipher data from the RHIC BES.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Automatic Building Energy Modeling (AutoBEM)

Principal Investigator: Joshua New, Oak Ridge National Laboratory

Co-Investigators: Piljae Im, Oak Ridge National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
300,000 node hours

Research Summary

There are approximately 124 million residential and commercial buildings in the U.S. consuming $395 billion per year in energy bills - 73% of the nation's electricity, approximately 80% during peak generation. DOE's Building Technologies Office (BTO) has the overarching goal to reduce energy use intensity (EUI) 30% by 2030 compared to a 2010 baseline. DOE's Office of Electricity (OE) has established the Grid Modernization Laboratory Consortium (GMLC) with the aim of making the nation's electricity grid more resilient as a foundational infrastructure supporting the Nation's security, economy, and modern way of life. This resilience is facilitated by achievements in energy storage to handle the challenges of decentralized generation toward dispatching load to match generation via intelligent buildings and devices. Despite progress, modeling suffers from high transaction costs necessary to create, refine, understand, and effectively utilize a building energy model.

BTO and OE/GMLC have co-funded the "Virtual EPB" project which has created a digital twin of 178,368 buildings (bit.ly/virtual_epb), empirically validated the virtual energy use from every building [in partnership with the Electric Power Board of Chattanooga, TN (EPB)], simulated nine monetization scenarios to quantify energy efficiency impacts on utilities and their ratepayers, and integrated results into EPB's operational business systems to quantify the sub-hourly, building-specific energy, demand, emissions, and cost impacts (bit.ly/AutoBEM). The Virtual EPB project continues to extend several software capabilities detailing the data sources and algorithms in the Automatic Building detection and Energy Model creation (AutoBEM).

This project will leverage existing organizational relationships, scalable data sources, and unique algorithms to attempt, for the first time, nation-scale building energy use. The team is currently working with companies to make the resulting building energy models and analysis free and publicly available to stimulate private sector activity towards more grid- aware energy efficiency alternatives for the built environment.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Electromagnetic corrections to strong dynamics

Principal Investigator: Amy Nicholson, University of North Carolina, Chapel Hill

Co-Investigators: Kate Clark, NVIDIA,
Michele Della Morte, Centre for Cosmology and Particle Physics Phenomenology, University of Southern Denmark,
Andrea Shindler, Facility for Rare Isotopes Beams, Michigan State University,
Andre Walker-Loud, Lawrence Berkeley National Laboratory,
Ben Hoerz, Lawrence Berkeley National Laboratory,
Henry Monge-Camacho, University of North Carolina

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

Lattice QCD (LQCD) is starting to deliver theoretical results to be confronted with experiments at an unprecedented level of precision. This is a fundamental pre-requisite to probe physics beyond the Standard Model (BSM). To control the precision of LQCD results at the order of, or below, the 1% total accuracy, it becomes unavoidable to introduce QED effects in LQCD calculations.

Standard methods for including electromagnetic interactions in LQCD calculations result in power-law finite-volume corrections to physical quantities. Removing these by extrapolation requires costly computations at multiple volumes. We have recently introduced a new and alternative method to regulate power-law finite-volume infrared corrections by introducing a photon with a non-vanishing mass. The modified QED action is dubbed QED_M.

The goal of this project is to provide a robust and theoretically sound lattice QED formulation that allows a control over all the systematics at the sub-percent level. To achieve this, we propose to extend our study of QED_M including dynamical quarks in the photon propagators and perform a comprehensive study of the volume and lattice spacing effects over a range of photon masses. We will use 7 LQCD gauge ensembles spanning 4 different pion masses (130, 180, 220, 310 MeV), 3 lattice spacings (0.15, 0.12, 0.09 fm) and values of mpi*L ranging from 4 to 9.

The proposed research is closely aligned with the goals of the 2015 Long-Range Plan for Nuclear Physics, specifically in the area of Nuclear Structure and Reactions. This proposal focuses on a necessary step towards the understanding of nuclear interactions mediated by QCD and the Electroweak theory.

Title: Chiral Nuclear Interactions from Nuclei to Nucleonic Matter

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Hadron Structure from Lattice QCD

Principal Investigator: Kostas Orginos, William & Mary

Co-Investigators: Christopher Monahan, William&Mary,
Balint Joo, Oak Ridge National Laboratory,
David Richards, Jefferson Laboratory,
Fank Winter, Jefferson Laboratory,
Jianwei Qiu, Jefferson Laboratory,
Anatoly Radyushkin, Jefferson Laboratory/Old Dominion University,
Savvas Zafeiropoulos,Marseille University, France

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

We propose to use the Oak Ridge Leadership Class Computing Facility's IBM/nVIDIA, Summit, to perform detailed numerical studies of hadronic structure. This work will provide essential theoretical support to the current (Jefferson Laboratory 12 GeV, BNL) and future Electron-Ion Collider (EIC) experimental program in hadronic physics.

In the last few years, a major achievement in hadronic physics has been the development of new methods that allow for direct computations of the longitudinal and transverse structure of hadrons. These groundbreaking developments allow, for the first time, the determination of the full longitudinal momentum-fraction depen- dence of parton distribution functions (PDFs) from lattice QCD, and thus opens up a new window for the theoretical study of the structure of the fundamental building blocks of matter, such as the pion and the nucleon. Experimentally, hadron structure studies are a central part of DOE's nuclear physics programs, both with current experimental facilities, such as the 12 GeV upgrade of Jefferson Lab, and at the future Electron-ion Collider. Furthermore, in the LHC era PDFs of the nucleon are essential input in the search of new physics and for discovering new heavy particles.

This project will explore these new methods to investigate the properties of the pion, the lightest hadron, and the nucleon. In particular, we will calculate the pion, kaon and nucleon Generalized Parton Distributions (GPDs) which describe the 3D structure, and the pion and kaon distribution amplitudes, revealing vital information about the quark and gluon degrees of freedom in these hadronic states.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Evolutionary Multi-scenario Simulation Environment for Autonomous Vehicle Testing

Principal Investigator: Robert Patton, Oak Ridge National Laboratory

Co-Investigators: Thomas Potok, Oak Ridge National Laboratory,
Laura Pullum, Oak Ridge National Laboratory,
Mark Coletti, Oak Ridge National Laboratory,
Shang Gao, Oak Ridge National Laboratory,
Jordan Chipka, General Motors,
Ajay Deshpande, General Motors

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
150,000 node hours

Research Summary

Autonomous vehicles (AV) continue to develop at an extraordinary pace. Low level autonomy already exists in production vehicles with prototypes, using higher level autonomy, currently being tested in specific cities. It is anticipated that the AV market size could be as much as $60 billion U.S. dollars by 2030. While success has been shown, existing vehicles have not achieved full autonomy. To continue the pace of development toward full autonomy, an advanced simulation environment based on high performance computing will be needed to effectively test the Artificial Intelligence (AI) that will be required for these vehicles. No methods currently exist for automatically generating, much less optimizing, driving scenarios for this purpose. This project plans to develop evolutionary optimization methods on the Summit system to design optimal driving scenarios for the testing and validation of AI-based vehicle control systems. The approach will enable extensive testing of AV with multi-scale scenarios (geographic locations, times of day, number of vehicles, pedestrians, miles driven, etc.). The research team has previously scaled several optimization methods for AI algorithms using 100% of both Titan and Summit. This project will build on this prior success, to quickly create a simulated testing environment that supports the creation of a fully autonomous driving system for the AV market.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Integrating HPC molecular simulation with neutron scattering to study complex biological systems

Principal Investigator: Loukas Petridis, Oak Ridge National Laboratory

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
300,000 node hours

Research Summary

Cells use dynamic, flexible structures to accomplish many tasks. Understanding cell function requires probing the shape and conformation of biological complexes and assemblies whose structure is neither rigid nor static. Many of the cellular molecular machines are multicomponent systems that transiently change state. Others are intrinsically disordered proteins - a class of proteins that plays an important role in signaling pathways. A major challenge is characterizing the structural flexibility of these proteins to correlate with their function, and dysfunction. This project will address this challenge with HPC simulation methods to gain a predictive understanding and support the development of computational pipelines for neutron science in advance of the Spallation Neutron Source Second Target Station (STS).

Development of high performance computing techniques that enable integration of neutron structural and dynamical information across multiple resolutions (and from other experimental techniques) will be key to providing on-line visualization and analysis of the structure and dynamics of complex biological systems at STS. Advanced tools that integrate theory, molecular dynamics simulations and scattering experiments will enable researchers to characterize the structural complexity of biological molecules relevant to improved biofuels and bioproducts. The team will simulate proteins associated with cellulose synthesis in plants and the membranes of bacteria. The computational models will be employed to develop a conceptual design for a small-angle neutron scattering instrument at the STS. This effort will demonstrate how integration of different modeling techniques can transform research of flexible bio-systems and be applicable to many other challenging systems.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Chiral Nuclear Interactions from Nuclei to Nucleonic Matter

Principal Investigator: Maria Piarulli, Washington University in St. Louis

Co-Investigators: Lorenzo Andreoli,Washington University,
Jason Bub, Washington University,
Garrett King, Washington University,
Saori Pastore, Washington University,
Alessandro Lovato, Argonne National Laboratory & Trento Institute for Fundamental Physics and Applications, Italy,
Noemi Rocco, Argonne National Laboratory & Fermi National Accelerator Laboratory,
Robert Wiringa, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
200,000 node hours

Research Summary

The microscopic approach to describe atomic nuclei and nucleonic matter relies on a theoretical description of individual interactions between protons and neutrons, and their interactions with external electroweak probes. Over the last two decades, chiral effective field theory has established itself as the method of choice to systematically construct nuclear many-body forces and electroweak currents that are rooted in the fundamental symmetries of quantum chromodynamics (QCD). In the present work, we plan to provide a comprehensive study of the model-dependence of the equation of state of neutron matter, particularly relevant in view of the recent detection of gravitational waves by the LIGO-Virgo collaboration. The equation of state of strongly interacting matter is sensitive to features of nuclear dynamics at short distances posing strong constraints upon the behavior of the microscopic Hamiltonians. Nuclear physics at short distances is dominated by short-range multinucleon correlations. Our understanding of their formation mechanisms and specific characteristics in nuclear systems is relevant not only to the role of QCD in generating nuclear forces but also to the physics of high-density nuclear matter that one expects to exist at the cores of neutron stars.

The calculations that we plan to carry out will be performed with the set of local Δ-full chiral nuclear potentials developed by our group, and Quantum Monte Carlo methods.

Title: DNS Simulations of Coolant Flow in the High Flux Isotope Reactor

Principal Investigator: Emilian Popov, Oak Ridge National Laboratory

Co-Investigators: Joseph Cambareri, North Carolina State University,
Igor Bolotnov, North Carolina State University

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
220,000 node hours

Research Summary

The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL) is a source of thermal and cold neutrons for research projects throughout the US used to study phenomena in numerous scientific and engineering disciplines. As part of the US Department of Energy (DOE) National Nuclear Security Administration's (NNSA) initiative to reduce the enrichment of research and test reactors, a research project is underway to investigate the conversion of HFIR from a high enriched uranium (HEU) core to a low enriched uranium (LEU) core. Due to the complex channel geometry and the difficulty of performing LEU testing and experiments, data supporting this conversion is highly limited. Therefore, high-fidelity numerical data is required to verify and calibrate Reynolds-Averaged Navier-Stokes models.

Direct numerical simulation (DNS) of turbulent single- and two-phase flows at a leadership computing facility allows for users to attain unprecedented level of detail and can answer fundamental questions about the interaction and evolution of turbulence within complex geometries. The highly detailed simulation of all turbulent structures using a DNS approach will allow for the collection of statistical information relevant to turbulent flow parameters, such as the turbulent kinetic energy, k-ε model constants and the Prandtl number required to enforce the correct wall heat transfer.

With the assistance of leadership computing facilities, detailed numerical data will be produced for the development of new closure laws to improve the prediction accuracy of computational fluid dynamics (CFD) models. These developments will help to capture turbulent flows in fine detail and facilitate the thermal-hydraulic design of HFIR and next generation energy systems.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Flow Physics and Machine Learning Based Modeling of SBLI in Transonic Compressors

Principal Investigator: Stephan Priebe, GE Research

Co-Investigators: Rathakrishnan Bhaskaran, GE Research,
Daniel Wilkin, GE Aviation,
Ramakrishnan Kannan, Oak Ridge National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
230,000 node hours

Research Summary

Shock/boundary layer interactions (SBLI) in transonic airfoils have significant impacts on the aerodynamics of turbomachinery. In the realm of commercial aircraft propulsion alone, it is estimated that the benefit of an improved physical understanding and predictive capability of SBLI would be of the order of 125 million gallons of jet fuel and 850,000 metric tons of greenhouse emissions for U.S. airlines every year.

This project will execute high-fidelity simulations of SBLI in a transonic turbomachinery airfoil. SBLI is difficult to predict accurately using standard design tools due to shortcomings in the underlying models. This effort will employ high-fidelity simulations to gain new physical insights through detailed post-processing, and apply machine-learning techniques to derive improved models trained on the high-fidelity simulation data. These models can provide an order of magnitude reduction in computational cost for engineering flows at relevant operational conditions, which are critical for guiding design of next-generation energy and propulsion machines.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Optimization studies of the LBNF - PIP-II complex for Megawatt beams on target

Principal Investigator: Igor Rakhno, Fermi National Accelerator Laboratory

Co-Investigators: Nikolai Mokhov, Fermi National Accelerator Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
450,000 node hours

Research Summary

The Deep Underground Neutrino Experiment and Long-Baseline Neutrino Facility (DUNE-LBNF) are under development at Fermilab since early 2010s. The primary scientific objectives of DUNE are to carry out a comprehensive investigation of neutrino oscillations to test CP violation in the lepton sector, determine the ordering of the neutrino masses, and to test the three-neutrino paradigm (electron, muon and tau neutrino). The LBNF will provide a 120-GeV proton beam on a neutrino production target utilizing a new 800-MeV superconducting Linac which is expected to be completed in 2027. The LBNF will provide neutrino fluxes and detector infrastructure at the near site (Fermilab) and far site.

The neutrino beamline, which utilizes a target and horn systems, decay pipe, hadron absorber and other systems, is a core component of the LBNF. At present—as a result of numerous iterations—there exists an optimized design with a 1.5-m graphite target and focusing system consisting of three horns. The design inherits experience from previous neutrino projects, in particular—NuMI at Fermilab (Neutrinos from Main Injector). Also, various energy deposition and radiological calculations have been performed for major components of the beamline, including the target itself, horns, decay channel, and hadron absorber. All such simulation studies are done by means of precise Monte Carlo modeling of radiation transport and interactions with matter in a broad energy region, utilizing the power and capabilities of the Fermilab's MARS code. A detailed MARS model of the PIP-II facility—both accelerator beamline itself and infrastructure—is developed. It is required for comprehensive Monte Carlo studies from the standpoint of radiation shielding including both normal operation and accident scenarios. The model should be verified, and test runs should be done. All that is a pre-requisite before performing numerous production runs.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Design of Next Generation Energy Conversion Systems using Extreme-scale Computing

Principal Investigator: Venkat Raman, University of Michigan

Co-Investigators: Venkat Tangirala & Sarah Monahan, GE Research;
Pete Strakey and Don Ferguson (DOE National Energy Technology Laboratory)

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
200,000 node hours

Research Summary

Gas turbines form the core of energy conversion devices used for aviation propulsion and stationary power generation. Traditional gas turbines, operating under a Brayton cycle, are approaching limited opportunities to improve thermal efficiency. Applying continuous detonations as the mode of combustion is a disruptive technological approach that can overcome this challenge, yielding decreased entropy generation and pressure rise. Based on open literature reported trade studies, thermal efficiency of such devices can reach the 67% target that DOE seeks, while reducing fuel consumption by 10-15%. One implementation of such detonation combustion is the rotating detonation engine (RDE), which has the potential to revolutionize gas turbine combustion technology by enabling high-efficiency power generation engines.

RDEs use a continuously moving detonation wave to process fuel-air mixture that enter the system. Emerging designs inject air and fuel through separate streams, and the effectiveness of the turbulent mixing process determines the detonation wave characteristics. As a result, injector design is a crucial element of RDEs. The focus of this project is to develop highly detailed simulations of practical RDEs to address two key design issues – stability and emissions. First, RDEs are highly sensitive to exit and inlet fuel/air boundary conditions. Hence, understanding the interaction of the detonation wave with these operating features is necessary to ensure stability and robustness of the device. Second, the high temperature and pressure inside the combustion chamber could impact NOx emissions. In particular, RDE injection design can have a first order impact. An analysis of the fluid mechanics of NOx formation is necessary in order to translate these combustors to practical gas turbines for power generation and other applications.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Earth System Simulations for Arctic Coastal Research

Principal Investigator: Andrew Roberts, Los Alamos National Laboratory

Co-Investigators: Joel Rowland, Los Alamos National Laboratory,
Luke Van Roekel, Los Alamos National Laboratory,
Mathew Maltrud, Los Alamos National Laboratory,
Nicole Jeffery, Los Alamos National Laboratory,
Ethan Coon, Oak Ridge National Laboratory

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
650,000 node hours

Research Summary

Coastal systems are some of the most complex and dynamic regions on Earth. Though only a small fraction of Earth's total area, these narrow bands around our continents are where terrestrial, marine, atmospheric, and human processes all interact, with significant ecological and economic consequences. In the Arctic, coastal systems are of disproportionate importance when compared to other parts of the globe. They modulate the input of heat, fresh water, and organic matter into the Arctic Ocean in ways that have the potential to generate globally significant feedbacks.

Two key factors make understanding of Arctic coastal systems an urgent and challenging national priority. First, with the loss of perennial sea ice and permafrost thaw, the Arctic has undergone arguably the largest physical transition of any region on Earth over the past several decades. Second, the Arctic coastal zone is at greater risk than other coastal zones in terms of environmental hazards and impacts of climate change on economic and resource development as well as national security. DOE has funded a new project focused specifically on modeling Arctic coastal environments, titled 'Interdisciplinary Research for Arctic Coastal Environments' (InteRFACE).

This project will support development, testing, and ensemble simulations using the Energy Exascale Earth System Model (E3SM), configured especially for InteRFACE with a regionally-refined Arctic ice-ocean mesh coupled to a standard resolution atmosphere. The InteRFACE simulation campaign will compared previous simulations to new ones that include landfast sea ice; a more accurate mixing scheme; and contributions of permafrost loss to river runoff.

Improvements to E3SM developed in InteRFACE will feed back into the main E3SM code base to alleviate strong polar biases that exist in the Arctic and sub-Arctic of the current version of the model. The project will also be designing and using innovative analysis tools to interpret new additions to the model.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: The gluonic structure of the proton

Principal Investigator: Phiala Shanahan, Massachusetts Instiutute of Technology

Co-Investigators: Artur Avkhadiev, Massachusetts Institute of Technology,
Daniel Hackett, Massachusetts Institute of Technology,
Patrick Oare, Massachusetts Institute of Technology,
Dimitra Pefkou, Massachusetts Institute of Technology

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

Understanding the structure of the proton in terms of the fundamental quark and gluon constituents encoded in the Standard Model of particle physics is a defining challenge bridging nuclear and particle physics research. In particular, while great progress has been made over the last decades to reveal the quark structure of the proton, very little is known about its gluon structure. With the planned construction of an Electron-Ion Collider (EIC) at Brookhaven National Laboratory as the highest priority for new construction in the Nuclear Science Advisory Committee long-range plan, significant experimental progress in developing a coherent picture of the gluon structure of the proton can be expected over the next decade. The key goal of the calculations outlined in this proposal is to obtain the first controlled predictions of aspects of the gluon structure of the proton relevant to this experimental program, providing critical information necessary for the development and optimization of the EIC by determining the kinematic regions that should be experimentally targeted and precision goals for key measurements. The project will also provide theory predictions and benchmarks for fundamental aspects of the proton's structure, such as its pressure distribution, ahead of first data-taking.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Atomistic Bridges to Carbon Defects @ Exascale

Principal Investigator: Ashley Shields, Oak Ridge National Laboratory

Co-Investigators: Jennifer L. Niedziela, Oak Ridge National Laboratory,
Sara B. Isbill, Oak Ridge National Laboratory

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
100,000 node hours

Research Summary

Due to their high strength-to-weight ratio, carbon fibers (CF) are increasingly used in high-performance applications, including improved fuel efficiency for transportation and in turbine blade manufacture for increased wind-energy generation. With such substantial impacts on the energy sector, the implications of a thorough understanding of defect-induced changes to the structural integrity of CFs are far reaching. It is therefore of fundamental significance to understand how these defects form during CF manufacture and use and their contribution to the tensile strength of the fiber. Experiments on defect formation and fiber failure can be monitored in situ using vibrational spectroscopies, namely Raman and infrared (IR). While a great deal is known about how Raman spectral responses are altered in the presence of different kinds of CF defects, Raman is a very inferential measurement, particularly in the limit where selection rules break down. To date, little to no work has been done on modeling the spectral response of CFs as this endeavor requires large system sizes to ensure defect-defect interactions are minimized, a large number of calculations to simulate experimental vibrational spectra, and highly accurate methods to predict phonon modes to achieve qualitative comparison with the experimental spectra. For this reason, the use of leadership class computing is essential.

The key goal of this work is to connect computational determinations of defect stability under equilibrium and non-equilibrium conditions to experimentally collected vibrational spectra obtained from Raman, IR, and neutron scattering. This project aims to bridge the current gap between experimental observations and an atomistic understanding of the impact of various types of CF defects on tensile strength and other material properties by utilizing highly scalable ab initio methods to generate a comprehensive understanding of the vibrational properties of CF analogues. Thermodynamically feasible defective CF structural units will be identified using density functional theory (DFT) calculations. For the most stable defects, the corresponding Raman, IR, and INS spectra will be calculated using both static and dynamic ab initio methods. The advantage of ab initio molecular dynamics (AIMD) is its inclusion of finite temperature and full spectral reconstruction. The atomic-scale understanding of CF defects, in conjunction with existing experimental datasets, will identify structure-property relationships which may be leveraged to tune the properties of CF for a multitude of materials science applications.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Supercomputing for Automotive High-temperature Alloy Design

Principal Investigator: Dongwon Shin, Oak Ridge National Laboratory

Co-Investigators: Sangkeun Lee, Oak Ridge National Laboratory,
J. Allen Haynes, Oak Ridge National Laboratory,
Adri van Duin,Pennsylvania State University

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

This project aims to support the modern design of high-temperature alloys for automotive propulsion applications funded by the Vehicle Technologies Office (VTO) under Energy Efficiency and Renewable Energy (EERE). This project has successfully demonstrated in the first year that a suite of state-of-the-art integrated computational materials engineering (ICME) software packages can significantly benefit from high-performance computing (HPC) resources for massive data acquisition. For example, first-principles calculations of nearly a thousand variants of supercells consisting of several hundreds of atoms, as well as hundreds of thousands of molecular dynamics simulations, can be completed within a week. This unprecedented pace of a large volume of high-quality data population has enabled rapid iteration of alloy design hypotheses generation/validation and coupling of physics in the context of materials data analytics. ORNL's world-class alloy design expertise and advanced characterization across multiple DOE national laboratories will actively support the proposed HPC ICME tasks. EERE VTO intends to continue the successful paradigm transition of the ICME from workstations/clusters to modern HPCs in the second year. The outcome of this project is to fill key knowledge gaps and reduce the timeframe from prototype high-temperature alloy development concepts to their real-world deployment.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Predictive Modeling of Nanoporous Materials and Multi-phase Systems (Consortium)

Principal Investigator: J. Ilja Siepmann, University of Minnesota

Co-Investigators: Jason Goodpaster,University of Minnesota

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
220,000 node hours

Research Summary

An interdisciplinary, collaborative team will use predictive hierarchical modeling and machine learning to accelerate the discovery and design of materials for a variety of energy-related applications. To this extent, the proposed ALCC consortium project is divided into four topics:

- Hierarchical screening and machine learning for adsorption and transport in nanoporous materials aimed at the discovery of materials with superior performance, including composite zeolite nanosheet/polymer, post-synthetically modified metal-organic frameworks (MOFs), and the development of machine-learning models for the prediction of mixture isotherms from single- component isotherms and/or spatial distributions of adsorption energies.
- First principles Monte Carlo and molecular dynamics simulations aimed at improving characterization of cation-containing nanoporous zeolites nanoporous zeolites, post-synthetically modified MOFs, and of γ-Al2O3/ZnO/ZIF-8 composite membranes.
- Molecular dynamics simulations of homogeneously stretched and bubbly water systems aimed at advancing knowledge for multi-phase flow through multi-billion particle simulations at micron length scale.

Improving the understanding and selection of nanoporous materials for separation and catalytic processes in the chemical, biorenewable, and petrochemical industries has tremendous societal benefits. The data obtained in this project will be disseminated through peer-reviewed publications, presentation at scientific meetings, and open-source databases.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Understanding the role of hierarchical correlations in solution-phase chemical separations

Principal Investigator: Lynda Soderholm, Argonne National Laboratory

Co-Investigators: Wei Jiang, Argonne National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
100,000 node hours

Research Summary

As part of a large-scale project to study chemical separation, we hypothesize that hierarchical structuring provides as-yet unrecognized entropic drivers impacting the process efficacy. Liquid-liquid extraction (LLE), a free-energy driven process in commercial use today for purification and isolation of a variety of base metals, precious metals, and rare earths. LLE provides an excellent model system for probing underlying forces governing the energy partitioning associated with hierarchical structuring. Through this proposal we are requesting computational time for large-scale molecular-dynamics simulations, the results of which constitute a critical component underpinning the success of our project objectives.

Progress to unravel this problem has been hampered by several factors, most notably the availability of experimental tools to probe multi-lengthscale solution correlations, limits on the size of systems that can be treated computationally, and the overall difficulty of treating such a multiple-component biphasic system. In order to make inroads into this problem we have recently begun a BES-funded machine-learning project to quantify multidimensional component correlations and their roles in LLE efficacy. We are attacking this problem using chemistry-aware neural-network approaches. We are amassing a wide range of chemical data, including analytical evaluation, characterization tools, synchrotron data, all to quantify molecular interactions in solution. The final component needed in our efforts to quantify LLE will come from large-scale molecular-dynamics (MD) simulations.

MD simulations provide critical input information to our machine-learning (ML) studies. First, they provide us metrics for the molecular-to-nanoscale solution correlations that can be compared with our experiments. The results from the MD simulations will provide insight to understand our experimental results through modeling. They will also allow us to quantify changes in structuring with changes in system. The MD simulations will transform the functions obtained as ML outputs into results that can be understood within the context of chemistry knowledge. We will perform high performance MD simulations with greatly scalable sampling method and high fidelity force field. It is expected that this approach will result in a new paradigm for the design of novel and robust chemical-separations processes.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: High-Fidelity Kinetic Modeling of Magnetic Reconnection in Laboratory Plasmas

Principal Investigator: Adam Stanier, Los Alamos National Laboratory

Co-Investigators: Jonathan Jara-Almonte,Princeton Plasma Physics Laboratory,
William Daughton, Los Alamos National Laboratory,
Ari Le, Los Alamos National Laboratory,
Robert Bird, Los Alamos National Laboratory

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
30,000 node hours

Research Summary

Magnetic reconnection is the process by which magnetic field-lines change their topology in highly conducting plasmas. It is one of the fundamental long-standing problems in magnetized plasma physics, occurring in a wide range of laboratory and space plasma environments.

Significant progress has been made in recent decades through the combination of laboratory experiments, kinetic modeling within 2D numerical simulations, and space-craft measurements. However, a number of key questions remain concerning the behavior of reconnection in 3D, the coupling to other instabilities and turbulence, and the coupling to the larger scale systems that supply the magnetic flux and drive the reconnection layer. These questions have motivated the construction of two new DoE Collaborative User Facilities – the T-REX experiment, part of the Wisconsin Plasma Laboratory User Facility, and the FLARE experiment at Princeton Plasma Physics Laboratory.

In this project, we propose to conduct 3D first-principles kinetic simulations of these two experiments using the VPIC Particle-In-Cell code at scale on Cori. These simulations will include all of the relevant physics – kinetic effects, plasma and neutral particle collisions, and realistic experimental geometry and drive coils. VPIC has been optimized to take advantage of the longer SIMD registers and many-integrated-cores architectures such as the Knights Landing (KNL) chips. It has demonstrated world class performance on Cori, as well as other machines based on the Knights Landing architectures (Trinity and Theta) for production runs of the type we propose. These numerical simulations will support a DoE Office of Science Opportunities in Basic Plasma Science grant to model reconnection in these laboratory experiments. We anticipate that these simulations will shed new light on the physics of magnetic reconnection, which will advance the capabilities of DoE User Facilities, and help to understand reconnection events in magnetic fusion energy devices and space plasmas.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Reconstructing Neutrino Data with the MicroBooNE Liquid Argon Detector

Principal Investigator: Andrzej Szelc, University of Manchester

Co-Investigators: E. Gramellini, Fermi National Accerlerator Laboratory
G. Cerati, Fermi National Accerlerator Laboratory
W. R. Ketchum, Fermi National Accelerator Laboratory,
E. Church, Pacific Northwest National Laboratory,
C. Adams, Argonne National Laboratory,
J. Spitz , University of Michigan,
P. Guzowski,University of Manchester

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
200,000 node hours

Research Summary

The aim of this project is to use High Performance Computing to reconstruct the full dataset of neutrinos from the NuMI beam using the MicroBooNE detector, to perform the most precise measurements of electron-neutrino interactions on argon, as well as interactions of neutrinos originating in Kaon decays-at-rest (KDAR) and searches for decays of Beyond the Standard Model particles. In the last few years Liquid Argon Time Projection Chambers (LArTPCs) have become the go-to detector in neutrino physics. They are employed to answer key questions in particle physics and cosmology: the search for a new, fourth, neutrino state via short-baseline oscillations in the Short-Baseline Neutrino (SBN) programme at Fermilab, and the international Deep Underground Neutrino Experiment (DUNE) measurement of CP violation in the neutrino sector, will all use LArTPCs. Both of these measurements will rely on precise measurements of electron neutrinos appearing, through neutrino oscillations, in a muon neutrino beam. Independent measurements of electron-neutrino interaction properties on argon, combined with measurements of KDAR neutrinos at well defined energies would be therefore greatly beneficial to the DOE-funded International Liquid Argon neutrino program at Fermilab. Finally, any new physics found in the form of exotic particles would have a huge impact on physics and the future of the neutrino and dark matter programmes.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Heating and Particle Energization in Quasi-Perpendicular Shocks

Principal Investigator: Jason TenBarge, Princeton University

Co-Investigators:

ALCC Allocation: National Energy Research Scientific Computing Center (NERSC)
24,000 node hours

Research Summary

Collisionless shocks are a grand challenge problem in plasma physics and have been the subject of study for more than six decades. A major unanswered question on this frontier is, how does a collisionless plasma transform flow energy into particle thermal energy? The development of a detailed understanding of shocks in plasmas has been a long standing goal of the broader scientific community, both as a fundamental physics process and because of its applicability to a wide variety of phenomena throughout the universe. To improve our understanding of plasma heating and distribution function dynamics in weakly collisional plasmas, we propose to study kinetic quasi-perpendicular shocks using fully kinetic Vlasov-Maxwell (VM) simulations. The simulation code, Gkeyll, to be employed in this endeavor leverages cutting-edge numerical techniques to model the particle distribution function evolution in greater detail than ever before. The Vlasov approach with a continuum velocity representation is free of restrictions imposed by reduced continuum and Lagrangian kinetic models often employed, e.g., gyrokinetics and particle-in-cell methods.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: QMC-HAMM: From the nanoscale to the mesoscale

Principal Investigator: Lucas Wagner, University of Illinois

Co-Investigators:

ALCC Allocation: Oak Ridge Leadership Computing Facility (OLCF)
362,000 node hours

Research Summary

A major theme of condensed matter and materials physics is the relationship between the microscopic behavior of electrons and nuclei to the emergent low-energy mesoscopic behavior of materials. Elucidating this relationship is a challenge, since the microscopic model requires advanced solution methods for many-body quantum mechanics, and the mesoscopic picture can be rather compli- cated. In complex materials, standard concepts at the mesoscopic level such as phonons, spins, and electron-like excitations can interact in complex ways which are difficult to access experimentally. The state of the art in creating mesoscopic models starting from the microscopic behavior is based on density functional theory (DFT) calculations. In recent years, modern machine learning techniques have been able to reproduce potential energy surfaces from standard DFT functionals to a very high accuracy; the accuracy potential energy surfaces can be limited by the underlying data. In quantum materials such as twisted bilayer graphene, interactions between electronic excitations can be critical to their behavior. To resolve the above issues, it is necessary to move beyond density functional theory and to base mesoscopic models on more accurate microscopic calculations. In this project, we will use quantum Monte Carlo calculations as a base for two high-impact projects which can benefit from the extra accuracy.

For high-pressure hydrogen, we will use the supported package QMCPACK to compute forces on the atoms both in the insulating, metallic phases, including impurities relevant to astrophysics and hydride superconductivity (e.g. helium and lanthanum). For graphene structural properties, we will use QMCPACK to investigate the interaction between twisted sheets. From those forces, we will apply machine learning techniques to fit the forces. This will result in a force field applicable to both metallic and insulating hydrogen, allowing for detailed simulations of the phase transition. The code is extremely portable and functions on GPUs.

This proposal is in support of the QMC-HAMM project, supported by the Department of Energy. Simulation data will be published as part of the project. The hydrogen data will support efforts to understand hydrogen at extreme conditions, including astrophysical observations and high temperature superconductivity in those materials. The graphene data will support efforts underway in many labs to understand the nature of electrons in twisted bilayer graphene. Both efforts will also provide a valuable reference data set for less accurate calculations, which will be used to improve the overall quality of materials modeling.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Plasma Surface Interaction Modeling

Principal Investigator: Brian D Wirth, University of Tennessee

Co-Investigators: David Bernholdt, Oak Ridge National Laboratory,
Aidan Thompson, Sandia National Laboratory,
Karl Hammond, University of Missouri,
Wahyu Setyawan, Pacific Northwest National Laboratory,
Ilon Joseph, Lawrence Livermore National Laboratory

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
318,000 node hours

Oak Ridge Leadership Computing Facility (OLCF)
155,000 node hours

National Energy Research Scientific Computing Center (NERSC)
30,000 node hours

Research Summary

The realization of fusion as a practical, 21st Century energy source requires improved knowledge of plasma surface interactions (PSI) 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 ITER divertor, to low energy, mixed H-He plasma exposure in the presence of impurity atoms including beryllium, nitrogen and neon. In particular, two tasks are envisioned that investigate the surface response following implantation of beryllium, helium and hydrogen into the tungsten divertor, as well as the underlying mechanisms controlling the reduced tritium permeation and retention observed in helium exposed tungsten.

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE – 2020 ALCC AWARD

Title: Toward the Future: High fidelity simulation for next Generation Nuclear Reactors

Principal Investigator: Yiqi Yu, Argonne National Laboratory

Co-Investigators:

ALCC Allocation: Argonne Leadership Computing Facility (ALCF)
208,000 node hours

Oak Ridge Leadership Computing Facility (OLCF)
300,000 node hours

Research Summary

This proposal aims at performing high fidelity simulation for the design of next Generation Nuclear Reactors. Our team will perform two series of high-fidelity calculations on flow and heat transfer behavior for Pebble Bed Gas Cooled Reactor and force fluctuation in 5x5, 4 Span Pin Bundle with Spacer Grid..

The first portion of the work focuses on the Xe-100, a pebble bed high-temperature gas-cooled nuclear reactor that is designed to be smaller, simpler and safer than conventional reactors. Better understanding of flow behavior and heat transfer mechanisms is of great interest and importance for the design of a pebble bed reactor. High fidelity simulation can save tremendous resources needed for experimental deployment. Large Eddy Simulation (LES) will be performed with Nek5000 to investigate local fluid fluctuations, which impact heat transfer and provide a benchmark for lower fidelity models (RANS and porous media) as well. The objective is to obtain a detailed temperature distribution for pebble bed reactor with a high degree of accuracy. The project will provide an integrated workflow for high fidelity simulation on pebble bed reactors, which can be further utilized for all kinds of pebble bed reactor designs from different vendors.

Additionally, the design of spacer grid is of great importance to nuclear fuel vendors for both generation III and generation IV Nuclear Reactors. In order to enhance fluid mixing while preventing vibrations, it is important to fully understand the resulting fluid forces exerted on the pins. Repetitive forces of certain frequencies can activate vibration modes of the long, cylindrical fuel pins, potentially resulting in fuel cladding failure. The intent of the present analysis is to simulate a 5x5, 4 span pin bundle with spacer grids using LES and RANS. This pin bundle matches experiments performed by Framatome. The computations will be carried out using Nek5000 for its demonstrated high fidelity and scalability. The LES data will be visualized to gain understanding of the specific flow structures resulting from the spacer grid. Comparison between the LES pressure fluctuation data and the steady and unsteady RANS results will require the development of comparison metrics in order to assess the ability of RANS to predict flow induced vibration.