Type: Renewal
Title: "Ab-initio Nuclear Structure and Nuclear Reactions"

Principal Investigator: Gaute Hagen, Oak Ridge National Laboratory
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Serdar Elhatisari, Karamanoglu Mehmetbey University
Stefano Gandolfi, Los Alamos National Laboratory
Gustav Jansen, Oak Ridge National Laboratory
Dean Lee, Michigan State University
Alessandro Lovato, Argonne National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Los Alamos National Laboratory
Petr Navrátil, TRIUMF
Thomas Papenbrock, University of Tennessee, Knoxville
Saori Pastore, Los Alamos National Laboratory
Maria Piarulli, Washington University in St. Louis
James Vary, Iowa State University
Robert Wiringa, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (693,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (500,000 Theta node-hours)

Research Summary: Atomic nuclei are strongly interacting, quantum many-body systems displaying fascinating properties. They exhibit emergent phenomena characteristic of large complex systems while at the same time being laboratories of most fundamental laws of nature. Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs.

Building on previous INCITE research, this project will employ advanced ab initio quantum many-body techniques coupled with applied mathematics and computer science methods to study a wide range of nuclei and to accurately describe the atomic nucleus from first principles. The team's predictions will complement DOE's major investments in forefront experimental facilities, including existing low-energy nuclear physics facilities, Jefferson Laboratory, neutrino experiments, and the forthcoming Facility for Rare Isotope Beams (FRIB) under construction at Michigan State University. Ultimately, results from this INCITE project will help support and guide new experiments, explain observed phenomena, and potentially propel the discovery of new laws of nature.

Type: New
Title: "Adaptive DDES of a Vertical Tail/Rudder Assembly with Active Flow Control"

Principal Investigator: Kenneth Jansen, University of Colorado Boulder
Co-Investigators: Michael Amitay, Rensselaer Polytechnic Institute
Jed Brown, University of Colorado Boulder
Alireza Doostan, University of Colorado Boulder
John Evans, University of Colorado Boulder
John Farnsworth, University of Colorado Boulder
Michel Rasquin, University of Colorado Boulder
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute
Cameron Smith, Rensselaer Polytechnic Institute
Philippe Spalart, The Boeing Company
Edward Whalen, The Boeing Company

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,000,000 node-hours)

Research Summary: This project seeks to advance detached eddy simulations in aerodynamic flow control. The simulations will exploit anisotropic adaptive unstructured grids to match mesh length scales precisely to solution requirements which, together with a solver that has already scaled to more than 3 million processes, will allow a dramatic advance in computational modeling and associated scientific and engineering insight.

Building on previous allocations, these simulations will compare, at high Reynolds numbers, synthetic and sweeping jets with 24, 1, and 0 active jets. These parameter variations reach one quarter magnitude of flight conditions, which will give critical insight required for Aurora to carry out the first-ever high-Reynolds-number delayed detached eddy simulatio. This project is economically motivated by the goal of redesigning control surfaces to reduce their size.

The vertical tail is sized to handle an engine-out condition which requires it to be much larger than what is needed for all other conditions in the flight envelope. The economic impact is directly related to the size of the stabilizer since it is a significant contributor to drag in cruise where much of the fuel is expended.

Type: New
Title: "Advances in Quark and Lepton Flavor Physics with Lattice QCD"

Principal Investigator: Andreas Kronfeld, Fermilab
Co-Investigators: Peter Boyle, Brookhaven National Laboratory
Norman Christ, Columbia University
Carleton DeTar, University of Utah
Aida El-Khadra, University of Illinois Urbana–Champaign
Christoph Lehner, Universität Regensburg & Brookhaven National Laboratory

Scientific Discipline: Physics: Particle Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (670,000 Summit node-hours)

Research Summary: Quantum Chromodynamics (QCD) is the component of the Standard Model of particle physics from which hadrons and atomic nuclei emerge. The only known systematically improvable way to treat the long-distance, strongly-coupled dynamics of QCD is a Markov chain Monte Carlo (MCMC) method, generating a sequence of lattice gauge-field configurations with importance sampling. The dependence of the lattice data on physical parameters, namely the quark masses, and the (unphysical) lattice spacing is controlled with effective field theories.

Kronfeld's team will address fundamental questions in elementary particle physics, or high-energy physics. Their calculations will directly support extensive experimental efforts in this field. They will use numerical simulations of lattice QCD, and in some cases, they also incorporate corrections from electromagnetism and the small difference in the up- and down-quark masses, because the precision of corresponding experiments requires these effects.

The calculations geared to high-energy physics are well aligned with the US strategic plan, spelled out in the report of the Particle Physics Project Prioritization Panel.

Type: New
Title: "Aero-Propulsive Real Gas Effects for Human-Scale Mars Entry"

Principal Investigator: Eric Nielsen, NASA Langley Research Center
Co-Investigators: Ashley Korzun, NASA Langley Research Center

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (770,000 Summit node-hours)

Research Summary: The entry, descent, and landing (EDL) systems for the United States' eight successful landings on Mars all relied heavily on extensions of technology developed for the Viking missions of the mid-1970s. To achieve human exploration on Mars, new approaches to EDL are necessary in order to support delivery of substantially larger payloads to the surface. The goal of this project is to further advance the understanding of retropropulsion physics for deceleration at Mars by quantifying the impact of real gas effects on vehicle aerodynamics during this phase of flight. This work directly supports NASA efforts to characterize environments and requisite computational modeling approaches to enable implementation of this technology into a flight vehicle.

Nielsen's project builds on successful Summit Early Science and INCITE campaigns from 2019, and data from this investigation will be used to continue building aerodynamics models for the powered descent phase of flight, with uncertainties quantified to include the impacts of chemistry. In support of inert gas (air) supersonic retropropulsion wind tunnel testing under the Aerosciences Evaluation and Test Capability Challenge Project, wind tunnel data will be combined with results from the present simulations to support assessment of the state-of-the-art for ground test and computational capabilities targeting the retropropulsion problem. When combined with prior perfect-gas simulation data generated on Summit in 2019, the limitations in subscale testing with inert simulant gases will be quantified for the first time.

Type: New
Title: "Approaching Exascale Models of Astrophysical Explosions"

Principal Investigator: Michael Zingale, Stony Brook University
Co-Investigators: Max Katz, NVIDIA
Alice Harpole, Stony Brook University
Ann Almgren, Lawrence Berkeley National Laboratory
John Bell, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Maria Barrios-Sazo, Stony Brook University
Kiran Eiden, University of California, Berkeley
Brian Friesen, Lawrence Berkley National Laboratory
Doreen Fan, Stony Brook University
Andy Nonaka, Lawrence Berkley National Laboratory
Don Wilcox, Lawrence Berkley National Laboratory
Jean Sexton, Lawrence Berkley National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (700,000 Summit node-hours)

Research Summary: Zingale's team will use Summit to advance their state-of-the-art simulations of two astrophysical environments: X-ray bursts (XRBs) and white dwarf (WD) mergers to unprecedented realism. Both of these are multiscale, multiphysics problems, relying on the coupling of hydrodynamics, magnetic fields, gravity, diffusion, and reactions to model the evolution of explosive astrophysical flows. The team's application code, Castro, has been tuned to efficiently run these simulations entirely on GPUs on the OLCF Summit machine at scale, and they are already producing scientific results. This INCITE allocation will allow them to complete several new studies on both of these problems, pushing the limits of their models, to help understand the underlying physical mechanisms in these events. They will also explore the details of convection in massive stars using our code MAESTROeX, which shares a common development model with Castro. Zingale's team's massive star calculations will be built up over the proposed period, and using MAESTROeX, they will model the final stages of convection in massive stars for much longer periods than currently possible. The calculations they proposed are only possible because of the GPU architecture on the OLCF Summit machine—the large speed-up they attain when using GPUs allows them to perform calculations that were simply not possible before Summit.

Type: Renewal
Title: "A Baseline for Global Weather and Climate Simulations at 1km Resolution"

Principal Investigator: Nils Wedi, European Centre for Medium-Range Weather Forecasts

Co-Investigators: Peter Dueben, European Centre for Medium-Range Weather Forecasts
Valentine Anantharaj, Oak Ridge National Laboratory
Peter Bauer, European Centre for Medium-Range Weather Forecasts

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (460,000 Summit node-hours)

Research Summary: It is one of the major sources of uncertainty for both weather and climate predictions that important features of the atmosphere, such as deep convection, cannot be resolved explicitly within existing weather and climate models due to the limited grid spacing of these models. Deep convection is seen as crucial in regulating the vertical redistribution of energy, momentum, and heat, and the community of weather and climate modeling is striving for the "quantum leap" of climate science to allow for long-range simulations of the global atmosphere at O(1 km) resolution that represent deep convection explicitly within the simulation.

In this renewed project, Wedi's team has completed the world's first seasonal timescale global simulation (November 2018 - February 2019) of the Earth's atmosphere with 1.4 km average grid-spacing using the power of Summit. They will work to produce a successful seasonal prediction of the Atlantic Hurricane season (August 2019 – November 2019) with the global storm-resolving IFS model at 1.4 km grid-spacing.

The team's very high-resolution global simulations will resolve how deep convection feeds back on global dynamics of the atmosphere on an annual timescale, thus providing a baseline reference and guidance for the worldwide weather & climate modelling community.

Type: Renewal
Title: "Closing, Evaluating, and Validating Multiphase Flow Models in Porous Medium Systems"

Principal Investigator: Cass T. Miller, University of North Carolina at Chapel Hill
Co-Investigators: Jan F. Prins, University of North Carolina at Chapel Hill
William G. Gray, University of North Carolina at Chapel Hill

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (370,000 Summit node-hours)

Research Summary: Multiphase porous medium systems arise routinely in natural and engineered systems and span applications in the geosciences, process engineering, and the biomedical field. However, traditional models for understanding these systems suffer from a lack of connection to the microscale, where the physics are better understood, than at the macroscale, where the models are formulated and solved. Miller's team seeks to bridge these two scales by using leadership-class computing to develop a new generation of multiphase flow models for porous medium systems.

A prior INCITE allocation resulted in a rigorous derivation and computational confirmation of a hysteretic-free equation of state involving capillary pressure that applies to both equilibrium and dynamic conditions; the establishment of the precision in thermodynamically constrained averaging theory (TCAT) variables as a function of domain size; a new evolution equation for the geometric orientation tensor; a promising approximation for the velocity of the fluid–fluid interface; the formulation of evolution and constraint equations for mean and Gaussian curvature; and substantial progress on computational confirmation of the new theoretical developments.

In this project, the team will develop a macroscale simulator implementing the new TCAT model and paving the way for rigorous evaluation and validation of the entire model and not just the component parts individually. The researchers anticipate that this work will hasten the development of a new generation of TCAT-model-based simulators yielding higher fidelity simulation of multiphase porous medium systems than is possible using current approaches.

Type: New
Title: "COMPBIO: COMbining deep-learning with Physics-Based affinIty estimatiOn"

Principal Investigator: Peter Coveney, University College London
Co-Investigators: Shantenu Jha, Rutgers University
Rick L. Stevens, University of Chicago

Scientific Discipline: Other: Other

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (125,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (100,000 Theta node-hours)

Research Summary: Since the outbreak of COVID-19, researchers around the globe have been attempting to develop drugs that target specific the viral protein that are vital for its propagation. However, the drug discovery process employed in the pharmaceutical industry typically requires about 10 years and $2-3 billion for a single new drug, which is obviously not useful in emergencies like this pandemic. Machine learning (ML) techniques are increasingly being used to overcome this bottleneck. Recent developments in deep learning (DL) allow generation of novel drug-like molecules in silico by extensive sampling of the chemical space of relevance. However, their reliability depends heavily on the training data available; when insufficient reduces their effectiveness. Fortunately, physics-based and ML methods are complementary and, hence, combining these two should provide a very efficient way to predict binding affinities.

Coveney's team will develop and implement a novel in silico drug design method coupling ML and physics-based methods. It is important to note that our workflow is already set up and functional on Summit. Candidates will be sampled from both a billion-compound synthetically accessible space (including Enamine REAL) and selected from the output of a DL generative algorithm. The selected compounds will be scored using physics-based methods based on the binding free energies calculated and this information then be fed back to the DL algorithm for active learning, thereby refining its predictive capability. This loop will proceed iteratively involving a variety of physics-based scoring methods with increasing level of accuracies at each step ensuring that the DL algorithm gets progressively more accurate in its predictions. Augmenting human intelligence with artificial intelligence (AI) by supplementing chemists' knowledge can substantially reduce the throughput time for exploring this huge chemical space and hence improve the efficacy of exploration of real and virtual chemical libraries. The ongoing COVID-19 crisis has exposed severe limitations in the current pharmaceutical mode of drug discovery and it is imperative to overturn it to urgently develop a drug. This project is designed to accelerate the required transformation.

Type: Renewal
Title: "Computational Modeling of Biomolecular Machinery in Nucleotide Excision Repair"

Principal Investigator: Ivaylo Ivanov, Georgia State University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (260,000 Summit node-hours)

Research Summary: Nucleotide excision repair (NER) is an essential genome maintenance pathway that detects and removes harmful DNA lesions resulting from exposure to environmental carcinogens, toxins, alkylating agents, reactive oxygen species and ultraviolet radiation. NER stands out among all DNA repair pathways for its ability to remove the widest array of structurally unrelated lesions. The need to process a wide variety of damaged sites has given rise to a remarkably complex molecular machinery.

Understanding the molecular mechanisms of NER is a grand challenge in biomedical science. Progress toward this goal has been hindered by the size, complexity and dynamic nature of the assemblies that accomplish NER. To overcome this critical barrier to progress, the project will employ integrative modeling methods, combining state-of-the-art computation with experimental data from cryo-electron microscopy (cryo-EM), site-directed mutagenesis, crosslinking mass spectrometry (XL-MS) and small angle X-ray scattering (SAXS) to elucidate the assembly, function and regulation of key NER complexes.

Specifically, the project will focus on transcription factor IIH (TFIIH) as the centerpiece of the NER machinery. Parallel computational and experimental advances will yield key insights into the structure, dynamics and function of NER complexes while making direct connection to genetic disease phenotypes. Success of the project will thus have major impacts - both in understanding disease etiology and in offering a structural framework to devise effective treatments.

Type: Renewal
Title: "Computational Studies of Correlated Quantum Materials"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Steven Johnston, University of Tennessee, Knoxville
Satoshi Okamoto, Oak Ridge National Laboratory
Gonzalo Alvarez, Oak Ridge National Laboratory
Thomas Schulthess, Swiss National Supercomputing Centre
Douglas Scalapino, University of California, Santa Barbara
Eduardo D'Azevedo, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (900,000 Summit node-hours)

Research Summary: Correlated quantum materials are key components to developing new technologies but require optimization to reach their full potential. Leveraging state-of-the-art numerical algorithms on Summit, Maier's team deploys advanced numerical methods to study the behavior of high-temperature (high-T_c) superconductors and quantum spin liquids (QSL). These include improved and accelerated algorithms including the dynamical cluster approximation (DCA), determinant quantum Monte Carlo (DQMC), and density matrix renormalization group (DMRG).

The overarching goal of this project is to understand, predict, and ultimately control the effects of correlations in quantum materials and thus help guide the design of new materials with optimized properties. To achieve this goal, Maier's team uses state-of-the-art numerical algorithms, including DCA, DQMC, and DMRG techniques, to carry out reliable and controlled simulations of realistic but reduced models of these systems. A particular emphasis for this project is to use these techniques to calculate the properties of quantum spin-liquids and superconductors—two representative classes of correlated materials—to determine the mechanisms responsible for their properties. For the unconventional superconductors, the team seeks to understand the respective roles of magnetic, charge, orbital, and lattice degrees of freedom in shaping pairing correlations. For the quantum spin liquids, they aim to understand materials proposed to realize the celebrated Kitaev quantum spin liquid.

Type: New
Title: "Deciphering the Mysteries of Hydrogen Bonding in Water"

Principal Investigator: Sotiris Xantheas, Pacific Northwest National Laboratory
Co-Investigators: Edoardo Apra, Pacific Northwest National Laboratory
Bo Peng, Pacific Northwest National Laboratory
Ajay Panyala, Pacific Northwest National Laboratory
Sriram Krishnamoorthy, Pacific Northwest National Laboratory
Karol Kowalski, Pacific Northwest National Laboratory
Dominika Zgid, University of Michigan
Niranjan Govind, Pacific Northwest National Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: Water is important for sustaining life on Earth by playing a central role in several chemical and biological processes in living organisms. Some of the unique properties of water have been attributed to the plethora of its anomalous macroscopic properties and the complex diagram that categorizes the phases of liquid water and ice. A fundamental understanding of the origin of the anomalies of its macroscopic properties and especially their connection to molecular level information has been long sought but is still missing. Central to this understanding are the properties of hydrogen bonds and the fleeting network they form in extended systems.

Using Summit, Xantheas and his team will simulate the X-ray photoelectron spectra of water aggregates and models of liquid water and ice at an unprecedented accuracy using SPEC's scalable Green's Function Coupled Cluster (GFCC) library. The effort will contribute to the understanding of the anomalous macroscopic properties of water, nature's universal solvent and indispensable agent for sustaining life on Earth. Supercomputer resources will be used to provide the link between molecular level information of aggregates of water molecules and the macroscopic structure of liquid water and ice.

Type: New
Title: "Design of Peptides and Proteins on Classical and Quantum Computing Hardware"

Principal Investigator: Vikram Mulligan, Flatiron Institute
Co-Investigators: Richard Bonneau, Flatiron Institute and New York University

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (800,000 node-hours)

Research Summary: Artificial proteins and peptides represent a powerful and versatile class of molecules. The sequence of amino acid building blocks in such a molecule uniquely determines the fold of the molecule, and the fold uniquely determines the molecule's function. Unfortunately, the sequence-fold-function relationship is one that is computationally challenging to untangle, due the vastness of both the possible sequence space and the possible conformational space.

This project aims to reduce the computational and energetic costs of producing successful peptide macrocycle drugs or industrial enzymes using two approaches. First, it will develop low-cost machine learning methods that can approximate the output of computationally expensive validation simulations, ultimately allowing users without access to large-scale resources to perform design and validation tasks on much more modest computing systems. Second, it will explore the use of quantum computing technologies as a means of solving the design problem at much lower energetic cost. This requires large-scale classical computing hardware both for carrying out quantum computing simulations during quantum algorithm development, and for performing computational validation of designs produced on current-generation quantum computing hardware.

Ultimately, this project aspires to decimate the computational and energetic cost of creating successful, computationally designed folding heteropolymers with useful functions in medicine and manufacturing, and to greatly enhance the accessibility of these computational design technologies to the scientific community.

Type: New
Title: "Direct Numerical Simulation of Separated Flow over a Speed Bump at Higher Reynolds Numbers"

Principal Investigator: Philippe Spalart, Boeing Commercial Airplanes (retired)
Co-Investigators: Ramesh Balakrishnan, Argonne National Laboratory
Aleksandr Obabko, Argonne National Laboratory
Misun Min, Argonne National Laboratory
Paul Fischer, University of Illinois at Urbana-Champaign

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (585,000 Summit node-hours)

Research Summary: The vast majority of aerodynamic flows (i.e. flows over wings and aerodynamic bodies including wind turbines) as well as flows in the atmospheric boundary layer, over complex terrain and urban canyons, share a common feature in that they are characterized by high Reynolds number (i.e. Re of 1.e06 to 1.e09), regions of mild to massive flow separation, and physical processes that depend on length scales that are too small to be resolved. Furthermore, despite advances in the development of Reynolds Averaged Navier-Stokes (RANS) turbulence models, their widespread industrial use, and their role as wall models in detached eddy simulations, the prediction of turbulent separated flows continues to be a major challenge. This severely paces Boeing's ability to simulate flows with sufficient accuracy prior to flight test, especially over high-lift systems.

In this project, Spalart's team is developing direct numerical simulation of fully turbulent flow over a "Speed Bump" at a Reynolds number that is twice as large as the current state of the art. The flow will be fully turbulent, unlike at the lower Re value; the boundary layer responds to pressure gradient and surface curvature, thus emulating an airplane high-lift system and leading to separation. This is a much-needed test case for RANS turbulence modeling.

Type: New
Title: "Disorder and Statistical Mechanics of Alloys and Functional Materials"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Valentino R. Cooper, Oak Ridge National Laboratory
Ka Ming Tam, Louisiana State University
Hanna Terletska, Middle Tennessee State University
Yang Wang, Carnegie Mellon University
Haixuan Xu, University of Tennessee, Knoxville

Scientific Discipline: Materials Science: Materials Discovery, Design, and Synthesis

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (200,000 Summit node-hours)

Research Summary: The goal of this project is a first principles based, quantitative understanding of alloys and functional materials beyond the ideal, zero temperature ground state. To achieve this goal, Eisenbach's team will combine density functional theory based ab initio calculations with statistical mechanics methods and first principles data driven models. The calculations for disordered materials, statistical sampling of configuration distributions and the generation of first principles data for model generation share as common features a high level data dependent stochastic part and a compute intensive deterministic kernel, that will allow the exposure of multiple levels of parallelism, scaling towards the exascale.

In this project the team will investigate partially overlapping classes of important material that are of significant from both a basic science point as well as for their potential technological applications. Solving the problems related to the first principles understanding of real materials poses challenges that require extraordinary computational capabilities. While the ground state properties of some pure compound can readily be calculated, real materials with defects and impurities and complex magnetic configurations have to be considered. This makes the calculation of even the ground state for realistic models containing approximately 100k atoms a petascale problem. Calculating the finite temperature properties of these materials requires orders of magnitude more computational resources. Finite temperature effects will be modeled by sampling the energy landscape with theWang-Landau (WL) statistical approach. The value of the energy at the sampled points will be determined by the Locally Self-consistent Multiple Scattering (LSMS) method. The efficiency of WL sampling, the speed of the LSMS, and the computing power of Summit combine to allow a truly first-principles thermodynamic description of magnetism and disordered materials.

Type: New
Title: "DNS and LES of Internal Combustion Engines to Understand Origins of CCV"

Principal Investigator: Sibendu Som, Argonne National Laboratory
Co-Investigators: Saumil Patel, Argonne National Laboratory
Muhsin Ameen, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Energy Efficiency

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,000,000 node-hours)

Research Summary: A key scientific challenge surrounding internal combustion engines (ICE) is the understanding, modeling, and control of cycle-to-cycle variability (CCV) in engine performance. CCV contributes to unevenness in the running of the engine, excessive engine noise and emissions, and engine knock, which can be potentially damaging. This project aims to develop a detailed understanding of the origins of CCV in a laboratory-scale modern engine using a combination of large eddy simulation (LES) and direct numerical simulation (DNS) techniques. While the high-fidelity LES will provide "gold-standard" data to understand root causes for CCV, the DNS will provide "ground truth" data for portions of the engine cycles to improve heat-transfer and combustion models further.

Establishing a progressive hierarchy of detailed simulation campaigns that will enable scientific discovery and development of predictive models, this project involves five main tasks: (1) Performing multi-cycle wall-resolved LES of a Direct-Injection Spark-Ignition (DISI) engine at motored conditions. (2) DNS of the compression strokes of a few select engine cycles to fully resolve the flow-field to assess the tumble breakdown process in more detail than have ever been captured before. (3) Wall-resolved LES with fuel injection to study the mechanism of momentum transfer between the fuel jet and the large scale in-cylinder tumble and swirl structures. (4) and (5) Multi-cycle, wall-resolved LES of the DISI engine at fired operating conditions for well-mixed and partially stratified operating conditions. The "gold-standard" LES and "ground truth" DNS datasets will be archived so that other researchers can access the data. The knowledge gained from this project will improve our understanding of ICE and help in developing more efficient and cleaner engines.

Type: New
Title: "DNS of Roughness Effects on Compressor and Turbine Performance and Heat Transfer"

Principal Investigator: Richard Sandberg, The University of Melbourne
Co-Investigators: Ivan Marusic, University of Melbourne
Tom Jelly, University of Melbourne
John Leggett, University of Melbourne
Aamir Shabbir, General Electric Aviation
Sriram Shankaran, General Electric Aviation

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (623,000 Summit node-hours)

Research Summary: Surface roughness affects fluid flow in many applications, from the atmospheric boundary layer, which always involves rough surfaces, to many engineering applications, where initially smooth surfaces may become rough due to fouling or erosion. An engineering application where roughness effects can significantly reduce efficiency (by up to 10% in several components) is the gas turbine (GT).

Understanding and predicting roughness effects in GT flows is particularly challenging because realistic roughness topologies from in-service engines can be very intricate and cannot easily be characterized by simple concepts, such as a sandgrain roughness. Also, the flow fields in GTs are highly complex. How the surface roughness interacts with and affects those phenomena is far from fully understood and no models exist that are generally applicable and accurate. Any engine performance improvements realized through better understanding and prediction of roughness effects can have a fuel-spend advantage of order billion-$, together with a significant CO_2 emission benefit.

Sandberg's team will leverage recent capability advances in performing first principle based simulations to improve our understanding and modeling of the intricate interactions of realistic surface roughness with the complex flow physics in gas turbines. The new knowledge and improved models will reduce fuel cost and emissions. The planned simulations are extremely computationally intensive and only possible by applying a highly efficient CFD solver, here HiPSTAR, developed by the PI and research group and extensively optimized for the GPU architecture of Summit, on a leadership computer facility.

Type: Renewal
Title: "Enabling the Design of Drugs that Achieve Good Effects without Bad Ones"

Principal Investigator: Ron Dror, Stanford University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (786,000 Summit node-hours)

Research Summary: Using massively parallel simulations on Summit, Dror's team is working to reveal how G protein–coupled receptors(GPCRs)—the largest class of drug targets—select which intracellular signaling proteins to activate. One-third of all existing drugs target G protein–coupled receptors (GPCRs), but designing effective, safe drugs for these receptors remains challenging. A major current effort in drug discovery involves a search for "functionally selective" ligands that promote signaling of a given GPCR through desired pathways while avoiding signaling through undesirable pathways responsible for dangerous side effects. The results of this project will enable development of medicines that elicit more desired effects with fewer side effects, providing a foundation for the design of safer and more effective treatments for a wide variety of diseases.

In a prior INCITE allocation, Dror's team made substantial progress toward this goal by identifying distinct conformations of a GPCR that have clear preferences for coupling to different intracellular signaling proteins (G proteins and arrestins). They also discovered how ligands can select for one conformation over another. They used these results to design ligands with desired signaling profiles, which have been validated by their experimental collaborators.

In this project, the team will continue focusing on identifying GPCR conformations that stimulate arrestin signaling more than G-protein signaling or G-protein signaling more than arrestin signaling. Determining such conformations is critical to enabling the rational design of GPCR-targeted drugs that achieve the desired effects with fewer side effects.

Type: Renewal
Title: "Energy Exascale Earth System Model"

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Peter Caldwell, Lawrence Livermore National Laboratory
Walter Hannah, Lawrence Livermore National Laboratory
Phil Jones, Los Alamos National Laboratory
Noel Keen, Lawrence Berkeley National Laboratory
L. Ruby Leung, Pacific Northwest National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Sarat Sreepathi, Oak Ridge National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,200,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (530,000 node-hours)

Research Summary: This INCITE project supports the Energy Exascale Earth System Model (E3SM) model, a multi-laboratory project developing a leading-edge climate and Earth system designed to address DOE mission needs.

Taking advantage of new leadership-class computing architectures, E3SM is now capable of simulations that resolve individual storms yet also run sufficiently long to separate climate signal from weather noise. Uncertainty in the parameterization of large convective storms has been identified as the primary source of uncertainty in climate predictions, so this advancement is expected to improve their accuracy.

E3SM will be used to compute climate sensitivity to elevated greenhouse gases. A global storm-resolving model configuration will be used alongside a novel hybrid multiscale modeling framework configuration that combines a storm-resolving model with conventional low-resolution global dynamics; the ultimate aim is to quantify the degree to which these new capabilities improve on the predictive power of conventional Earth system models.

Type: Renewal
Title: "Exascale Artificial Intelligence to Accelerate Scientific Discovery"

Principal Investigator: Robert Patton, Oak Ridge National Laboratory
Co-Investigators: Thomas Potok, Oak Ridge National Laboratory
Steven Young, Oak Ridge National Laboratory
Catherine Schuman, Oak Ridge National Laboratory
Travis Johnston, Oak Ridge National Laboratory
Seung-Hwan Lim, Oak Ridge National Laboratory
Maxim Ziatdinov, Oak Ridge National Laboratory
Sergei Kalinin, Oak Ridge National Laboratory
Joel Saltz, Stony Brook University
Derek Rose, Oak Ridge National Laboratory
Bill Kay, Oak Ridge National Laboratory

Scientific Discipline: Computer Science: Computer Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (300,000 Summit node-hours)

Research Summary: Many scientific research applications rely on the analysis of imagery produced using scientific instruments such as microscopes. This analysis benefits from neural networks because, unlike other computer vision approaches, this approach does not rely on hand-engineered features. Instead, neural networks learn the features needed for the image-processing task from the data.

In this project, Patton's team is developing scalable artificial intelligence systems to accelerate understanding of two different application areas: (1) nanoscale material fabrication using scanning transmission electron microscopy (STEM) imagery and (2) cancer research and treatment using digital pathology imagery.

The results of this work could bring real-time, image-based feedback for STEM significantly closer to a reality and enable the linking of pathology images and cancer registry abstracts to create a unique, population-wide, molecular view of cancer.

Type: New
Title: "Exascale Simulation of Topological Materials Dynamics"

Principal Investigator: Prineha Narang, Harvard University

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (470,000 Summit node-hours)

Research Summary: Materials are known to be topological when their electronic band structures show mathematical properties that can be linked to quantized electronic responses. In a wide range of chemical compounds, the low-energy behavior is readily explained by topological field theories that provide a high-level approach and a transparent way to understand many exotic material properties. Within this past decade, a number of material systems have been theoretically identified and experimentally verified to exhibit topological properties. Of particular interest are magnetic Weyl semimetals and more exotic structures, which show a phase transition and a collective mode for temperature and pressures that modify the topological properties dynamically.

Narang's team will use Summit to make exascale calculations of dynamics, both storing (ultralarge-scale memory) and accurately (GPU-accelerated large-scale) computing the scattering matrices to understand the physical properties of topological quantum matter at room temperature. This work in computational condensed-matter has the potential to revolutionize an astonishing range of applications, from optoelectronic energy conversion to quantum information processing.

Type: New
Title: "Extreme Scale Multiphysics Models to Predict Metastatic Tumor Cell Fate"

Principal Investigator: Amanda Randles, Duke University

Scientific Discipline: Biological Sciences: Medical Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (290,000 Summit node-hours)

Research Summary: Cancer is the attributed cause of death in one in four cases in the United States and metastasis, a complex multistep process leading to the spread of tumors, is responsible for more than 90% of these deaths. Circulating tumor cell (CTC) survival in the bloodstream plays a key role in future arrest and seeding of metastatic sites and this survival is strongly influenced by exposure to varying hemodynamic forces, a mechanistic understanding of the shear forces experienced by a CTC or cluster of CTCs as it moves through the body and how that relates to cell survival remains an elusive goal. Current research efforts to uncover these mechanisms are fundamentally driven by in vitro and in silico experiments. One of the greatest challenges in this experiment-rich era of cancer research has been the ability to effectively analyze this information and isolate root causes of exhibited behaviors. Randles's team of computational researchers has complemented wet lab inquiry with high-resolution, fluid-structure-interaction simulations to address biomedical questions. The team's long-term goal is to establish an open source, easily extensible software tool to provide access to such methods in a way that allows even cancer researchers with limited coding experience to effectively complement their data with in silico enquiry to target individual properties in a way that wet lab approaches alone cannot achieve.

Predicting the trajectory of cancer cells through the body requires capturing system-level transport at cellular resolution which pushes the limits of today's supercomputers. To overcome this challenge, Randles's team has developed a new method that couples physics-based models across these different scales and leverages a hybrid CPU-GPU approach to maximize performance. Through algorithmic advances that efficiently use hardware on the Summit supercomputer and seamlessly integrate both multi-scale and multi-resolution models, the team established a finely resolved window with explicitly resolved cells to track a cancer cell through a large arterial network. They seek to leverage their novel, multiphysics algorithm that enables biomedical researchers to capture cell-specific phenomena over the long length-scales seen in the microvasculature or larger geometries to investigate properties influencing cell fate in complex vasculatures.

Type: Renewal
Title: "Extreme-Scale Simulations for Advanced Seismic Ground Motion and Hazard Modeling"

Principal Investigator: Christine Goulet, University of Southern California
Co-Investigators: Yifeng Cui, San Diego Supercomputer Center
Philip Maechling, University of Southern California
Kim Olsen, San Diego State University
Doriam Restrepo, Universidad EAFIT
Yehuda Ben-Zion, University of Southern California

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (319,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (480,000 Theta node-hours)

Research Summary: Accurate seismic hazard assessments help inform and prepare society for earthquakes, enabling the development of design and mitigation strategies that save lives and reduce economic losses in the event of a major earthquake. The advancement of earthquake modeling and simulation tools is critical to reducing uncertainties and improving the accuracy of seismic hazard assessments.

With this INCITE project, researchers from the Southern California Earthquake Center (SCEC) are working to enhance their earthquake simulation and hazard mapping tools to provide the best possible information in terms of earthquake ground motion and seismic hazard. This involves extending the SCEC software ecosystem, including CyberShake, for example, to the next level of fidelity by advancing its capabilities to resolve shaking estimates and related uncertainties across a broadband range of frequencies of engineering interest (i.e., 0–20 Hz). To enable the computation of broadband seismic hazard maps, the team will improve their computational codes' ability to accurately simulate high-frequency shaking. A significant part of the research involves the integration and testing of new and improved simulation elements in the codes to model topography, realistic material rheology and inelasticity, and the stochastic representation of the heterogeneous portions of the Earth's crustal structure. It will also require the development of new processing workflows to address the added complexity. The larger simulation domains, higher resolution grids, and new physics models implemented in their codes will pose new challenges that can only be addressed with DOE's leadership-class computing resources. The modeling enhancements in the SCEC software ecosystem will increase the accuracy of simulations, reduce scientific uncertainties, and broaden the usefulness of these software tools in engineering applications.

Type: New
Title: "Fermi Surface of Plutonium: Fundamental Insight into Electronic Correlation"

Principal Investigator: Gabriel Kotliar, Rutgers University
Co-Investigators: Corey Melnick, Brookhaven National Laboratory
Sangkook Choi, Brookhaven National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (385,000 Summit node-hours)

Research Summary: Plutonium has been referred to as "an element at odds with itself," and "a physicist's dream and a metallurgist's nightmare." Consternation with and excitement for plutonium arise because its properties defy description by the traditional tools of solid-state physics. For example, the standard implementations of density functional theory (DFT) underestimate the volume of the cubic phase (δ-Pu) by about 30% and spin-DFT predicts that δ-Pu, a paramagnetic material, has a large magnetic moment. That is to say, DFT cannot even predict the most basic properties of plutonium. Turning towards experiment is also challenging: plutonium is extremely toxic and famously radioactive. Dynamical mean field theory (DMFT) and its combination with DFT (DFT+DMFT) were developed in part to address these problems, and this approach was successful: DFT+DMFT simulations accurately predicted many material properties of plutonium for the first time, and these simulations provided substantial insight into the electronic structure of plutonium. Accompanying this insight was the development of the predictive theory of strongly correlated materials. Indeed, plutonium is a paradigmatic strongly correlated material, and advancing our understanding of this system also advances our ability to understand and describe strong correlations themselves.

Kotliar's team will conduct DFT+DMFT simulations of three archetypical plutonium materials of practical and fundamental interest, α-Pu, δ-Pu and $PuCoGa_5$. They will compute their Fermi surfaces for the first time using state-of-the-art software they have developed for this purpose. These simulations will provide invaluable guidance for upcoming experiments at Los Alamos National Laboratory, and, as the Fermi surface is a central quantity in the foundational theories of condensed matter physics, they will also provide important insight into plutonium and its paradigmatic electronic correlations. This insight, which cannot be gained by applying the traditional tools of condensed matter physics, will lead towards a better understanding of those exciting applications like superconductivity which strong correlations manifest.

Type: New
Title: "First-Principles Simulation of Electronic Stopping Excitation and Beyond"

Principal Investigator: Yosuke Kanai, University of North Carolina at Chapel Hill
Co-Investigators: Andre Schleife, University of Illinois Urbana-Champaign

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,900,000 node-hours)

Research Summary: Electronic stopping describes the transfer of kinetic energy from highly energetic charged particles to electrons in matter. This process results in massive electronic excitations within the target material.

Although the researchers' first-principles simulation approach—based on non-equilibrium real-time time-dependent density functional theory (RT-TDDFT)—has brought great success to modeling electronic stopping of ion projectiles like protons and alpha-particles in various matters, there are additional challenges to overcome. With this project, the researchers intend to advance their approach so as to study electronic stopping processes of complex systems for which going beyond typical-linear response theory formalism is necessary.

In particular, this work aims (1) continue to investigate electronic excitations in solvated DNA under ion irradiation (i.e. protons, alpha-particles, and carbon ions) in the context of ion beam cancer therapy, and (2) advance the researchers' first-principles method for studying non-linear electron dynamics and how excited electrons promote defect diffusion in semiconductors under proton, electron, and photo irradiation.

Type: New
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Shantenu Jha, Rutgers University
Daniel Peter, King Abdullah University of Science and Technology
Matteo Turilli, Rutger University

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (550,000 Summit node-hours)

Research Summary: Information about Earth's interior comes from seismograms recorded at its surface. Seismic imaging based on spectral-element and adjoint-state methods has enabled assimilation of this information for the construction of 3D (an)elastic Earth models. These methods account for the physics of wave excitation and propagation by numerically solving the equations of motion and require the execution of complex computational procedures that challenge the most advanced high-performance computing systems.

Tromp's project addresses the long-standing challenge of imaging Earth's interior at the global scale based on full-waveform inversion. The team combines 3D simulations of global seismic wave propagation with the assimilation of seismographic data from an exhaustive earthquake catalog. These simulations will result in a much improved Earth model with drastically sharper contrasts around regions of interest. An anticipated impact on community paradigms includes sophisticated GPU-enabled open-source software freely distributed to the seismological community via the Computational Infrastructure for Geodynamics.

Type: New
Title: "High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics"

Principal Investigator: Choongseock Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Mark Adams, Lawrence Berkeley National Laboratory
Luis Chacon, Los Alamos National Laboratory
R. Michael Churchill, Princeton Plasma Physics Laboratory
Michael Cole, Princeton Plasma Physics Laboratory
Stéphane Ethier, Princeton Plasma Physics Laboratory
Robert Hager, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Seung-Hoe Ku, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado
Aaron Scheinberg, Jubilee Development
Mark Shephard, Rensselaer Polytechnic Institute
Sarat Sreepathi, Oak Ridge National Laboratory
Benjamin Sturdevant, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,300,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (900,000 node-hours)

Research Summary: This project uses use the gyrokinetic particle-in-cell code XGC to study two fundamental edge physics issues critical to the success of ITER and the magnetic fusion energy programs: (1) understanding and thus promoting innovative ways to achieve the transition from low- to high-confinement mode operation; and (2) a high-enough plasma edge pedestal in the high-mode with a wall heat-flux density below the material limit.

Achieving ITER's goal of a 10-fold energy gain depends critically on resolving these two issues. The nonlocal, multiscale, nonlinear plasma physics across the open and closed magnetic field geometries, which demand unstructured triangular mesh and neutral particle recycling, make the problem an extremely large one that requires trillions of marker particles for ITER.

Based on previous INCITE allocations, for physics the project will focus on the large-size effect (compared to the ion gyroradius) in the Fusion Power Operation phase (FPO) of ITER and in future magnetic-fusion reactors.

Type: New
Title: "High-fidelity Study of Turbulent Aeroacoustics in Open Rotor Propulsion"

Principal Investigator: Trevor Wood, GE Research
Co-Investigators: Stephan Priebe, GE Research
Aamir Shabbir, GE Aviation
Kishore Ramakrishnan, GE Research
Daniel Tweedt, GE Aviation
Trevor Goerig, GE Aviation
Syed Arif Khalid, GE Aviation

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (146,000 Summit node-hours)

Research Summary: There is a societal and regulatory need to substantially reduce utilization of fossil fuels and production of toxic emissions associated with aircraft propulsion, along with reductions in aircraft noise to curb the effects of both increasing air traffic and population density near airports. In recent years, GE has been developing a propulsion architecture that promises to revolutionize commercial aviation in offering a step change improvement in efficiency (over 10% fuel savings approximately, which would have been worth over 2.4% of airlines' direct operating costs in 2019 for example) while maintaining the high flight speeds we enjoy and expect today – the open rotor engine. Drawing from a rich history from the Unducted Fan (UDF®) program in the 80s to more recent work with NASA, FAA and partners in CFM (Safran Aircraft Engines), GE now aims to optimize open rotors for higher levels of fuel savings and simultaneously quieter noise levels generated by turbulent flow associated with the fan blades.

Only with the combination of the high fidelity simulation of turbulence with high-end supercomputing can GE more accurately address the complexities of the turbulent flow aeroacoustics features of open rotor design. Fully three-dimensional boundary layer flow physics, flow separation, and wake and vortex mixing requires a higher degree of prediction accuracy than is possible with conventional turbulence models. Using Large Eddy Simulation (LES), we can simulate these essential flow physics and their relation to the fan blade design. Wood's team will provide first-of-its-kind high-fidelity simulations for open rotor aeroacoustics, broadening the industrial reach of high performance supercomputing applications to accelerate development of this critical technology, ultimately enabling better design optimization while informing future modeling improvements.

Type: Renewal
Title: "High-Speed Turbulence with Shocks over Non-Adiabatic and Flexible Walls"

Principal Investigator: Johan Larsson, University of Maryland
Co-Investigators: Ivan Bermejo-Moreno, University of Southern California

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,800,000 node-hours)

Research Summary: This project investigates how supersonic wall-bounded turbulent flows are affected by the thermal wall boundary condition and how they interact with flexible walls. High-fidelity simulations at different Mach numbers, Reynolds numbers, and imposed wall temperatures will be used to create a database that advances the theoretical description of how the mean velocity profile scales with these factors. As current theories fail at high Mach numbers for either strongly cooled walls or nearly adiabatic walls, the results of this work will be used to develop a predictive model that remains accurate across all flow conditions. This, in turn, will lead to improved modeling techniques for near-wall turbulence and improved semi-empirical friction.

This project also considers the interaction between supersonic turbulent boundary layers and shock waves in the presence of rigid and flexible walls, and will create highly resolved reference data for several such cases, including cases with crossflow that create skewed mean velocity profiles. These data will be used to assess and validate modeling techniques for near-wall turbulence in the context of large eddy simulations.

Type: New
Title: "Large-Scale Simulations of Light-Activated Matter"

Principal Investigator: Giulia Galli, University of Chicago and Argonne National Laboratory
Co-Investigators: Marco Govoni, Argonne National Laboratory
Francois Gygi, University of California, Davis

Scientific Discipline: Materials: Microscopic

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,200,000 node-hours)

Research Summary: This project carries out large-scale quantum simulations of light-activated processes in materials so as to tackle two classes of problems: the design of (1) sustainable materials that efficiently capture and convert solar energy, and (2) materials to build novel, optically addressable quantum platforms, including quantum sensors.

Simulations of electronic excited state properties of heterogeneous materials—including defects and interfaces—couple first-principles molecular dynamics and electronic structure methods beyond density functional theory, as implemented in the Qbox and WEST open-source code.

This work simulates point defects in wide band gap semiconductors for the realization of qubit and quantum sensors, as well as assemblies of nanostructured building-blocks that are present. It will deliver predictions of the structural and electronic properties of heterogeneous systems to be compared against experiment so as to obtain an integrated mechanistic understanding of the interaction of defective and nanostructured materials with light, in addition to validated data for systems of interest for sustainability and quantum technologies.

Type: New
Title: "Long Term 3D Simulations of Core-collapse Supernovae"

Principal Investigator: William Hix, Oak Ridge National Laboratory
Co-Investigators: Stephen Bruenn, Florida Atlantic University
James Harris, Oak Ridge National Laboratory
Eric Lentz, University of Tennessee
Anthony Mezzacappa, University of Tennessee

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (900,000 Summit node-hours)

Research Summary: Core-collapse supernovae, the explosive final moments of massive stars, are complex, dynamic, multi-physics events yielding a bright and energetic explosion from the birth of a neutron star or black hole. The central engine of a core-collapse supernova generates rare transient signals in gravitational waves and neutrinos. The explosion creates and ejects many chemical elements, including the primary constituents of the Earth, dominating the production of elements from oxygen to iron throughout the Universe. The core-collapse supernova problem has been a computational challenge for several decades, and today we are entering an era where the well-resolved, symmetry-free, three-dimensional (3D) simulations with sufficient physical detail and coupling necessary to understand these complex stellar explosions and their byproducts are now possible. However, the number of extant 3D simulations with adequate physics is small and none have been run until the explosion matures more than a second after the proto-neutron star forms.

Hix's team will run state of the art simulations that extend through all of the element creation process that occur in these supernovae to better understand the elements made. The 3D supernova simulations proposed here have two goals. First, the team seeks to understand the impact of stellar rotation on the explosion mechanism of core-collapse supernovae and the associated observables. Second, they seek to understand the development of the proto-neutron star wind following the onset of explosion.

Type: New
Title: "Mechanisms and Structure-based Evolution of Function in Eukaryotic Substance Transport"

Principal Investigator: Harel Weinstein, Weill Cornell Medical College of Cornell University
Co-Investigators: George Khelashvili, Weill Cornell Medical College of Cornell University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (691,000 Summit node-hours)

Research Summary: With computational simulations, Weinstein's team seeks to address the grand challenge of understanding fundamental molecular mechanisms of cell communication. They are studying a family of molecular machines transporting solutes across cell membranes in the human brain to learn how to modulate their activities in disease and create a molecular engineering template for chemical energy-driven molecular machines.

In this project, Weinstein's team will use advanced mechanistic analyses of trajectories from molecular dynamics (MD) simulations at unprecedented sampling scales to seek the needed level of understanding of complex biological functions, and to enable designs of synthetic analogs of molecular machines with specifically engineered properties and functions.

The team's workflows, already working on Summit, are continually optimized to take advantage of exceptional performance and efficiency of the MD software, of the adaptive algorithms for iterative convergence tests, and the analyses executed automatically on Summit. This enabled us to complete successfully the data collection from a job running on 1000 nodes of Summit, taking advantage most efficiently of (i)-Summit's GPU architecture by deploying massive swarms of independent simulations, and (ii)-the integration of our computational protocol and advanced workflows we implemented on Summit.

Type: New
Title: "Million Atom Chemical Dynamics at Heterogeneous Aqueous Interfaces"

Principal Investigator: Roberto Car, Princeton University
Co-Investigators: Lin Lin, University of California, Berkeley
Athanassios Panagiotopoulos, Princeton University
Annabella Selloni, Princeton University

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (720,000 Summit node-hours)

Research Summary: Molecular processes in aqueous solutions in contact with solid interfaces are central to geochemistry, biology, and energy technologies. Car's team is working to better understand these phenomena, which would make a significant step towards better controlling them, an issue of substantial societal impact. Computational modeling, specifically the use of Summit, is essential to accomplish this task because complexity and disorder makes it difficult to extract precise microscopic information from experiments.

Car's team will use Summit to model millions of molecules at the level of quantum mechanics for tens of nanoseconds. They will perform ground-breaking molecular dynamics simulations to study mass/charge transfer processes at a prototypical interface of titania (TiO_2) with aqueous solutions of varying pH and excess salt concentrations. The deep potential molecular dynamics (DPMD) method, developed at Chemistry in Solution and at Interfaces (CSI), makes use of modern artificial intelligence techniques to learn from accurate but costly quantum mechanical calculations the complex way in which the energy and charges of a multi-atom system depend on the system coordinates. By harnessing the computational power of Summit, DPMD makes possible million-atom simulations for time spans of up to hundreds of nanoseconds, while retaining quantum mechanical accuracy essential for modeling chemical dynamics. The proposed simulations will use 1 million water molecules and 100 thousand TiO2 units with varying acid (HCl), base (NaOH), and excess salt (NaCl) concentrations, to study how the pH gradients affect the ionic charge distributions in the solution and at the solid interface.

Type: New
Title: "Multi-ion Turbulence in Burning Plasma Experiments"

Principal Investigator: Emily Belli, General Atomics
Co-Investigators: Jeff Candy, General Atomics
George Fann, Oak Ridge National Laboratory
Gary Staebler, General Atomics

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (450,000 Summit node-hours)

Research Summary: Developing a fusion reactor relies on understanding the physics of self-sustaining or burning plasmas. A power-producing fusion reactor will require a well-confined plasma with high temperature and moderate density. Plasma confinement is limited by slow particle and energy loss due to turbulence driven by unstable plasma waves. Understanding this turbulence in burning plasma scenarios is thus essential to designing a tokamak fusion reactor like ITER – the next-generation burning plasma experiment, designed to produce a ten-fold return on energy – with optimal confinement properties.

Belli's team will use complex multi-ion simulations to model energy losses due to turbulent transport and maximize fusion performance. The simulations will model the cross-species interactions between the deuterium and tritium fuel ions, fusion helium ash impurity, wall impurities (beryllium and tungsten), and electrons. The mechanisms that drive the ion transport (including heavy tungsten ions) will be studied for high-confinement mode (H-mode) operating scenarios in both the central core, which is dominated by ion-scale turbulence, and in the outer core/edge, where multiscale turbulence (which spans ion to electron scales) exists. These simulations are particularly challenging because of the need to resolve the long space and time scales of high-Z impurities together with the short space and time scales of the much lighter electrons.

Type: New
Title: "Multi-Messenger Astrophysics at Extreme Scale in Summit"

Principal Investigator: Eliu Huerta, NCSA/University of Illinois at Urbana-Champaign

Co-Investigators: Roland Haas, NCSA/University of Illinois at Urbana-Champaign
Elise Jennings, Irish Center for High-End Computing
Tom Gibbs, NVIDIA
Max Katz, NVIDIA
Jeff Larkin, NVIDIA
Junqi Yin, Oak Ridge National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (145,000 Summit node-hours)

Research Summary: Astrophysical sources that may be contemporaneously heard in gravitational waves, seen in electromagnetic waves, and felt with cosmic neutrinos—Multi-Messenger Astrophysics— have radically transformed the landscape of theoretical physics and observational astronomy. Tens of gravitational wave sources detected to date have provided ample observational evidence for the existence and merger of black hole binaries; neutron star collisions have been identified as the engines that power short gamma rays bursts, and have provided the first glimpse of matter at supranuclear densities. Upgraded and new scientific facilities for Multi-Messenger Astrophysics will drive a major scientific revolution within the next decade.

With improved and new observatories, the number of Multi-Messenger sources will increase by orders of magnitude whereas available compute resources to enable discovery may remain the same or, as seen in practice, may even contract as science teams repurpose compute resources at their discretion. Therefore, a paradigm shift in computing and data, inspired by breakthroughs in the big data revolution is urgent and critical.

Huerta's team will combine physics-inspired, interpretable AI models and extreme scale computing to create the first generation of production scale, AI algorithms to enable novel data-driven discovery methodologies for Multi-Messenger Astrophysics.

Type: Renewal
Title: "Novel Methods for Complex Excited-State Phenomena in Functional Materials"

Principal Investigator: Jack R. Deslippe, Lawrence Berkeley National Laboratory
Co-Investigators: Steven G. Louie, University of California, Berkeley; Lawrence Berkeley National Laboratory
Jeffrey B. Neaton, University of California, Berkeley; Lawrence Berkeley National Laboratory
James R. Chelikowsky, University of Texas, Austin
Felipe H. da Jornada, Lawrence Berkeley National Laboratory
Diana Y. Qiu, Lawrence Berkeley National Laboratory; Yale University
Sivan Refaely-Abramson, Weizmann Institute of Science
Marina Filip, University of Oxford

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)

Research Summary: Many of the present technologies on which global industries are based, such as silicon technology for computers or optoelectronics and photovoltaics, will become increasingly more advanced with the advent of new technologies that are based on devices built from complex and functional materials. These new devices represent a broad class of systems which exhibit unique and controllable electronic and optical properties triggered by atomic arrangements specifically engineered at the nanoscale level.

Deslippe's team is applying and advancing state-of-the-art ab initio approaches to understand and predict complex excited-state phenomena in novel and functional materials. The team will explore various types of systems of structural complexity and emerging scientific interest to understand the underlying interactions dominating their optoelectronic properties and the structural dependencies of those interactions, thus identifying principles to rationally design new materials with optimal properties.

Type: Renewal
Title: "Nuclear Matter Dynamics in Real Time and the Heaviest Elements in Nature"

Principal Investigator: Aurel Bulgac, University of Washington
Co-Investigators: Piotr Magierski, Warsaw University of Technology
Kenneth Roche, Pacific Northwest National Laboratory
Nicolas Schunck, Lawrence Livermore National Laboratory
Kazuyuki Sekizawa, Niigata University
Ionel Stetcu, Los Alamos National Laboratory
Gabriel Wlazłowski, Warsaw University of Technology

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (300,000 Summit node-hours)

Research Summary: Nuclear physics is poised to answer fundamental questions about nature, but these questions are complex and the answers require the latest developments in theory, high-performance computing, and new emerging compute elements and architectures.

Bulgac's team is using the full quantum mechanical predictive tools needed to quantitatively describe nuclear fission, collisions of heavy ions, and fusion—including the total kinetic energy released, the properties and excitation energies of the fission fragments, their masses, charges, excitation energies, angular momenta, the spectra of emitted neutrons, the multinucleon, and the energy transfer in low and medium energy heavy-ion collisions.

The microscopic description of low-energy heavy-ion reactions, in particular the calculation of fusion cross-sections and of nucleon transfer cross-sections, has fundamental and practical importance. These reactions are relevant for the physics at the Facility for Rare Isotopes Beams and many other laboratories in US and across the world for further pursuing the quest for superheavy elements, for extending the periodic table of elements, and for explaining the origin and the abundance of chemical elements in the Universe.

Type: Renewal
Title: "Petascale Simulations of Kinetic Effects in IFE Plasmas"

Principal Investigator: Frank Tsung, University of California, Los Angeles
Co-Investigators: Warren Mori, University of California, Los Angeles
Han Wen, University of Rochester

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,800,000 node-hours)

Research Summary: Inertial fusion energy (IFE) devices hold incredible promise as a source of clean and sustainable energy, but there are significant obstacles to obtaining and harnessing IFE in a controllable manner.

A comprehensive model of laser-plasma instabilities (LPI) is crucial to the success of any IFE scheme, but one so far remains elusive. The physics involved in these processes (including both wave-wave and wave-particle interactions) is complex and highly nonlinear, necessitating the use of nonlinear kinetic computer models, such as fully explicit particle-in-cell (PIC) simulations. The ultimate goal—a long-standing challenge—is a constructed hierarchy of kinetic, fluid, and other reduced description approaches capable of modeling full spatial and temporal scales. Kinetic modeling has not yet yielded sufficiently complete understanding across the array of scales necessary to make strong connections with more approximate models and experiments.

The INCITE project is harnessing the power of DOE leadership computing resources to study the kinetic evolution of LPI on meaningful spatial and temporal scales directly relevant to various IFE scenarios. Using the popular PIC code OSIRIS, the team is performing fully kinetic simulations that will help advance research at the National Ignition Facility and other IFE experiments (e.g., direct drive and shock ignition studies at the OMEGA facility at the University of Rochester).

Type: Renewal
Title: "PlasmaMirrors 'in Silico': Extreme Intensity Light Sources and Compact Particle Accelerators"

Principal Investigator: Jean-Luc Vay, Lawrence Berkeley National Laboratory
Co-Investigators: Henri Vincenti, Commissariat à l'Energie Atomique
Axel Huebl, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (165,000 Summit node-hours)

Research Summary: Relativistic plasma mirrors (PM), produced when a high-power laser hits a solid target, can provide very promising compact sources of relativistic electron, ions, and very intense extreme ultraviolet Doppler harmonic light sources.

This project aims to show, in silico and using massively parallel pseudo-spectral particle-in-cell (PIC) simulations, that such PMs can provide a simple and common elegant solution to three long-standing challenges of ultrahigh-intensity (UHI) physics.

These three challenges are: (1) Can we produce high-charge compact electron accelerators with high beam quality that will be essential to push forward the horizons of high energy science? (2) Can we produce efficient and very compact high-energy ion accelerators to democratize cancer hadron-therapy? (3) Can we reach extreme light intensities approaching the Schwinger limit of approximately 10^{29}W·cm^{-2}, beyond which light self-focuses in vacuum and electron-positrons pairs are produced?

Type: New
Title: "Precision Calculations of Matrix Elements for Novel CP Violation Experiments"

Principal Investigator: Rajan Gupta, Los Alamos National Laboratory
Co-Investigators: Tanmoy Bhattacharya, Los Alamos National Laboratory
Vincenzo Cirigliano, Los Alamos National Laboratory

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: The standard model (SM) of elementary particles, including the recent understanding of neutrino masses and mixing, has been extremely successful in describing all phenomena up to the TeV scale probed at the Large Hadron Collider (LHC) in Geneva. At the same time new, and as yet unknown, physics is required to explain three profound mysteries: the observed matter-antimatter asymmetry of the universe, dark matter and dark energy. A profound mystery is the almost total absence of antimatter in the observed universe, whose explanation requires much larger violation of charge-conjugation-parity (CP) symmetry than exists in established theory.

Gupta's team will calculate the form factors (the momentum dependent strength of the coupling of neutrinos to nucleons) for the neutrino experiments, and the matrix elements of CP violation operators that give the size of their contribution to the neutron electric dipole moment. These calculations will increase the reach of experiments searching for novel CP violation in the neutrino sector and in neutron electric dipole moment.

Type: New
Title: "Predicting Ion Transport Kinetics at Complex Interfaces for Energy Storage"

Principal Investigator: Brandon Wood, Lawrence Livermore National Laboratory
Co-Investigators: Tae Wook Heo, Lawrence Livermore National Laboratory
Liwen Wan, Lawrence Livermore National Laboratory
ShinYoung Kang, Lawrence Livermore National Laboratory
Boris Kozinsky, Harvard University
Nicole Adelstein, San Francisco State University

Scientific Discipline: Materials: Macroscopic

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (640,000 node-hours)

Research Summary: The most promising high-capacity, solid-state energy storage systems—including next-generation batteries and hydrogen storage materials—rely on fast transport kinetics of ions. Computer simulations play an increasingly visible role in probing ion transport, generally employing idealized models to minimize computational cost and complexity. However, real components contain interfaces between different phases or grains, which can impact ion transport in unexpected and often problematic ways. The chemical and structural disorder at these interfaces is an exceptionally challenging problem to tackle using conventional approaches, instead requiring extensive multiscale simulations capable of spanning broad ranges of time and length scales.

Focusing on solid-state battery electrolytes and metal hydride hydrogen storage materials, this project integrates three sets of multiscale simulation capabilities to predict ion transport kinetics at interfaces. Large-scale quantum simulations are validated using computationally generated spectroscopic data to generate interface models. These models are then used to train dynamics simulations that can span a much larger range of configurations. Finally, the atomic-scale data are interfaced with a microstructure model that can incorporate complex interface arrangements present in real materials.

The multiscale simulations will be used to probe the relationship between physicochemical interface properties and ion transport kinetics, guiding rational engineering strategies for improving performance of advanced materials for grid and vehicular energy storage.

Type: New
Title: "Predictive Simulations of Phase Transitions in Dynamically Compressed Materials"

Principal Investigator: Ivan Oleynik, University of South Florida
Co-Investigators: Anatoly Belonoshko, Royal Institute of Technology, Sweden
Stan Moore, Sandia National Laboratories
Aidan Thompson, Sandia National Laboratories
Mitchell Wood, Sandia National Laboratories

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (300,000 Summit node-hours)

Research Summary: Oleynik's team will study fundamental mechanisms and kinetics of phase transitions in materials subjected to very high multi-Mbar pressures and multi-kK temperatures in the High Energy Density (HED) regime. Solid materials subjected to dynamic compression under such conditions created in the laboratory by powerful lasers and pulsed-power machines undergo phase transitions to complex solid and liquid structures, exhibiting unusual and exotic physics. Uncovering the fundamental HED physics of phase transitions in materials is of great importance for successful realization of inertial confinement fusion, understanding of origin and evolution of planetary interiors and National Nuclear Security.

The understanding of phase transitions at HED conditions is the urgent need for better control of hydrodynamic instabilities during inertially confined fusion (ICF) implosion of ablative materials, which critically depend on lack of heterogeneities in outer layer. These heterogeneities are due to the possible appearance of multiple solid and liquid phases during the first shock compression stage of the multi-shock laser pulse. Quantitative information on solid-solid and solid-liquid phase transitions of alternative ablative materials such as silicon carbide at multi-Mbar pressures and multi-kK temperatures is still lacking and urgently sought for in design of ICF experiments (targets and drive pulses) using hydrodynamic simulations of implosion.

By effectively utilizing the unprecedented power of the OLCF Summit supercomputer, this project aims to make transformative advances in understanding of fundamental physics of phase transitions under dynamic compression and guiding future experiments to confirm the predictions of our simulations.

Type: Renewal
Title: "Quantum Simulations of Photosystem II and Cuprate Superconductivity"

Principal Investigator: Shiwei Zhang, Flatiron Institute; College of William & Mary
Co-Investigators: Richard Friesner, Columbia University
David Reichman, Columbia University
Steven White, University of California, Irvine

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (552,000 Summit node-hours)

Research Summary: Predictive calculations in many-body systems governed by the laws of quantum mechanics represent a grand challenge in science. The combination of methodological developments and the advent of petascale and exascale computing presents a unique opportunity to make fundamental progress on this problem. The project of Zhang's team concerns two transition-metal oxide systems crucial to energy science: the catalytic site of Photosystem II (PSII) and cuprate high-temperature superconductors (HTSC).

PSII is a protein complex in plants that converts water to oxygen with high efficiency using light and has the potential to serve as a functional model for how solar energy can be harvested in order to perform useful work. The proposed computational and theoretical investigations aim to supplement experimental findings to provide a complete understanding of the structure, function, and mechanism of PSII. This will facilitate the design of artificial analogs with similarly high catalytic efficacy.

HTSC materials have the potential to revolutionize many energy-related technologies. However, the underlying physics is not well understood. Going beyond simple models, Zhang's team plans to produce more accurate physical predictions via direct calculations of the chemically realistic copper oxide system. The effort aims to bring about key insights towards the solution of a long-standing problem, provide a benchmark for simpler models, and explore a path to the rational design of new materials.

Type: New
Title: "Search for the QCD Critical Point"

Principal Investigator: Swagato Mukherjee, Brookhaven National Laboratory
Co-Investigators: Dennis Bollweg, Bielefeld University, Germany
Jishnu Goswami, Bielefeld University, Germany
Prasad Hegde, Indian Institute of Science, India
Frithjof Karsch, Bielefeld University, Germany
Peter Petreczky, Brookhaven National Laboratory
Philipp Scior, Bielefeld University, Germany

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (250,000 node-hours)

Research Summary: Strong interaction, a fundamental force of nature, is responsible for nearly the entire mass of our visible universe. Lattice QCD calculations of conserved charge fluctuations provide a sensitive probe of the phase structure of strong-interaction matter. Increasing theoretical evidence, based on such calculations, and experimental measurements of high order cumulants of such fluctuation observables, coming from the Beam Energy Scan (BES) at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory, suggest that a possible critical point (CEP) in the phase diagram of strong-interaction matter, is likely to be located at rather low temperature, $T < 140$ MeV, and high net baryon-number densities. This calls for further, high statistics large-scale hot-dense lattice QCD calculations, in the poorly explored low temperature, high density region. Most promising probes for the phase structure of strong-interaction matter and the search for a CEP are non-Gaussian cumulants of conserved charge fluctuations. These cumulants 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. Extracting information on these cumulants at rather low temperature and high net baryon-number densities, however, does require approaches that go beyond the commonly used approximation schemes, which are based on straightforward Taylor expansions or analytical continuation from numerical calculations at imaginary values of the baryon chemical potential.

By simulating the theory of strong interaction using the nation's fastest supercomputer, Summit, Mukherjee's team will predict its various phases. Their predictions will provide important guidance to experimental explorations of these phases in particle colliders.

Type: New
Title: "Simulating Collapsar Accretion Disks and Luminous Transitional Disks"

Principal Investigator: Alexander Tchekhovskoy, Northwestern University
Co-Investigators: Rodrigo Fernandez, University of Alberta
Francois Foucart, University of New Hampshire
Dimitrios Giannios, Purdue University
Daniel Kasen, Lawrence Berkeley National Laboratory
Matthew Liska, Harvard University
Philipp Moesta, University of Amsterdam

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (300,000 Summit node-hours)

Research Summary: Unleashing the GPU power of the Summit supercomputer, Tchekhovskoy's team will address two longstanding problems or science goals: how do dying massive stars, or collapsars, produce heavy elements, such as gold and platinum?, and how does radiation cause black hole feeding disks of gas to clump up and transition to a new luminous state? Addressing these problems is enabled by the fusion of the team's GPU-accelerated H-AMR code with the unparalleled power of Summit's GPUs. Both goals push the limits of physics and computation in preparation for future exascale systems and capitalize on the paradigm-shifting results recently obtained by the group.

Through previous allocations, Tchekhovskoy's team has worked to explore new frontiers in black hole physics by making a factor of 10 leap in resolution that is currently possible only on ORNL's Summit supercomputer. In this new project, they will carry out the next-generation simulations, which include radiation and neutrino transport, and enable direct attacks on long-standing problems previously thought inaccessible to first-principles studies.

Type: New
Title: "Stratified Turbulence at Very Low Froude Number"

Principal Investigator:	Stephen de Bruyn Kops, University of Massachusetts, Amherst
Co-Investigators:	James Riley, University of Washington Colm-Cille Caulfield, University of Cambridge Gavid Portwood, Lawrence Livermore National Laboratory

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:

Site:	Oak Ridge National Laboratory
Machine (Allocation):	IBM AC922 (260,000 Summit node-hours)

Research Summary: Stably stratified turbulence (SST) is a model flow for understanding fluid flows that are highly intermittent and anisotropic at large scales. The understanding derived from SST is important for applications ranging from climate modeling, to pollution mitigation, to deep sea mining, to military operations over cold land or ice. SST is also valuable for enhancing fundamental turbulence theory on turbulent/non-turbulent interfaces, internal intermittency, and anisotropic multi-scale energetics. In all turbulent flows, dynamic range, or the ratio of the largest the smallest length scales, has a profound effect on the fluid dynamics. Dynamic range is characterized by the Reynolds number, Re. SST, though, is at least a two parameter problem with Re characterizing the overall dynamic range and Froude number, Fr, describing the range of comparatively large length scales strongly affected by buoyancy.

Thanks in a large part to a DoD HPCMP Frontier award in 2014-18, de Bruyn Kops's research group has made significant progress in understanding flows with high Re and moderately low Fr [1-5]. The largest of these simulations were run on 15360 x 15360 x 7680 grid points. It has been hypothesized, though, that the dynamics of SST are fundamentally different if Fr is very low [6, 7]. This hypothesis has not been explored in detail because no researchers, to date, have had the computational resources and expertise to do so.

With this project, de Bruyn Kops and team will advance understanding and modeling of stratified turbulence and the dynamic range required to understand this region of parameter space, specifically 24000 x 24000 x 6000 grid points. This simulation size is practicable on Summit, which means that Summit enables us to cross a cusp in terms of turbulence dynamic range and understand a fluid flow regime not currently accessible for research by other methods.

Type: New
Title: "Toward the Design of Photonic Protein Crystals"

Principal Investigator: Sharon C. Glotzer, University of Michigan

Scientific Discipline: Materials Science: Materials Discovery, Design, and Synthesis

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: Photonic crystals are materials that exhibit unique properties in their interaction with light. The properties and behavior of crystalline materials depend directly on the quality of the crystals, which in turn depends on how the crystal formed. In this project, Glotzer's team will combine protein design and photonic property prediction to design biological photonic materials, which have a wide variety of applications for transparency, camouflaging, protection, sensing, and signaling.

Summit is an essential resource to carry out this research, which will allow the team to explore a large dataset of proteins with enough docking trajectories (fundamental to assembly trajectories) to investigate the general behavior of protein dimerization. This research will provide fundamental insight into the importance of shape complementarity in protein self-assembly and provide guidance to protein interface engineering.

Summit is also critical for exploring the enormous space of all possible photonic band structures, which depends on crystal structure and the dielectric properties of the constituents. Calculating a single band spectrum is computationally expensive but tractable on a single CPU core. Doing so for millions of design possibilities is considerably more challenging. Machine learning approaches such as this involve large datasets and large amounts of training that require tuning and exploration of hyperparameter spaces to be done correctly and therefore can only be carried out using leadership class machines.

Type: Renewal
Title: "Towards a Definitive Model of Core-Collapse Supernova Explosions"

Principal Investigator: Adam Burrows, Princeton University
Co-Investigators: Joshua Dolence, Los Alamos National Laboratory
David Radice, Princeton University
Michael Aaron Skinner, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 node-hours)

Research Summary: Core-collapse supernovae dramatically announce the death of massive stars and the birth of neutron stars. During this violent process, a combination of high-density nuclear physics, multi-dimensional hydrodynamics, radiation transport, and neutrino physics determines whether and how the star explodes.

This project explores the full physics of supernova explosions. Researchers are using the state-of-the-art, highly scalable, 3D radiation-hydrodynamics simulation code Fornax to determine the explosion energies, neutron star residual masses, and ^{56}Ni and ^{44}Ti yields—all as functions of progenitor mass.

A solution will benefit ongoing efforts of observers and instrument designers in the U.S. and around the world engaged in projects to determine the origin of the elements, measure gravitational waves, and interpret laboratory nuclear reaction rate measurements in light of stellar nucleosynthesis.

Type: Renewal
Title: "Towards Predictive Simulations of Functional and Quantum Materials"

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Anouar Benali, Argonne National Laboratory
Olle Heinonen, Argonne National Laboratory
Jaron Krogel, Oak Ridge National Laboratory
Ye Luo, Argonne National Laboratory
Lubos Mitas, North Carolina State University
Miguel Morales, Lawrence Livermore National Laboratory
Eric Neuscamman, University of California, Berkeley
Fernando Reboredo, Oak Ridge National Laboratory
Luke Shulenburger, Sandia National Laboratories

Scientific Discipline: Materials Science: Microscopic

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,200,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 node-hours)

Research Summary: The goal of this project is the prediction and understanding of quantum-mechanical properties of materials that display novel properties including novel quantum phases. These materials are of outstanding fundamental scientific interest and present the potential for the development of new sensors and devices.

In all of the materials studied, small changes in composition, pressure, strain, doping, and applied field yield greatly altered properties, which is a challenge to simulation and modeling. This project therefore applies approaches based on Quantum Monte Carlo (QMC), as implemented in the open-source QMCPACK code. By directly solving the Schrödinger equation and by treating the electrons at a consistent highly-accurate many-body level, these methods can be applied to general elements and materials, while employing very few approximations.

Supported by the DOE BES Computational Materials Sciences Center for the Predictive Simulation of Functional Materials and core BES programs, this project operates alongside experimental collaborators to enable joint theory-experimental work.

Type: Renewal
Title: "Towards Understanding Instability Mechanisms of Axial Compressors"

Principal Investigator: Charles Hirsch, Numeca International

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: Energy transformation systems rely on rotating machines, such as gas turbines, transforming chemical energy from combustion into mechanical energy, to efficiently drive electrical generators or aircraft engines. Their impact on the environment is significant and reduction of emissions and fuel consumption are critical to the continued growth and sustainability of the global energy conversion process. Key factors in the reduction in emissions and fuel consumption are tied to the performance of the gas turbine components, namely compressor, combustor and turbine components and their operating range.

The present project is focused on compressor performance limits, which condition the stability and operating range of the whole of the gas turbine system. Of particular interest is the mechanisms leading to the onset of stall and the subsequent appearance and propagation of rotating stall configurations in axial compressors.

This knowledge will help industrial turbomachinery designers understand and potentially delay or avoid the onset of stall, resulting in components with robust stall margins and operating ranges with higher efficiency. In addition, by collecting and feeding these new data towards design methodologies based on engineering methods, either empirical or Reynolds-averaged Navier-Stokes equations, optimizations with enhanced knowledge and significant potential energy savings will be made possible.

The industrial partners Dresser-Rand and Concepts NREC are contributing to the data analysis and to the potential integration of the gained knowledge into their design process and design tools.

Type: Renewal
Title: "Ultrafast Control of Functional Materials"

Principal Investigator: Priya Vashishta, University of Southern California
Co-Investigators: Rajiv Kalia, University of Southern California
Aiichiro Nakano, University of Southern California

Scientific Discipline: Materials: Microscopic

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,600,000 node-hours)

Research Summary: Recent advancements in ultrafast materials science have raised the possibility of using picosecond light pulses to switch emergent material properties on demand in various functional materials. Such ultrafast and high-quantum-efficiency switching of material properties (e.g., polarization and conductivity) has the potential to revolutionize future information and energy technologies. With this INCITE project, researchers from the University of Southern California leverage leadership-scale quantum dynamics simulations, machine learning, and x-ray free-electron laser (XFEL) experimental data to extend the frontier of ultrafast materials science.

State-of-the-art XFEL and ultrafast electron diffraction (UED) experiments now provide unprecedented capability to observe light-induced material dynamics with sub-nanometer spatial and sub-picosecond time resolutions. By observing the motions of electrons and atoms at their natural time scales, these experiments help accelerate ultrafast control of quantum-material properties. Understanding the complex far-from-equilibrium quantum dynamics from first principles, however, poses an enormous computational challenge that necessitates the use of leadership computing resources.

Building on the success of previous INCITE awards, the University of Southern California team is using the Theta supercomputer to predict ultrafast function-property-structure relationships that dictate light control of emergent material properties in complex nanostructures composed of three classes of advanced functional materials: (1) layered-material heterostructures and magic-angle heterostacks; (2) novel chalcogenide perovskites; and (3) topological skyrmions superlattices. The researchers are performing 10^4-atom nonadiabatic quantum molecular dynamics (NAQMD) and billion-atom reactive molecular dynamics (RMD) simulations that not only mirror far-from-equilibrium electronic and lattice dynamics in next-generation XFEL experiments at the forthcoming Linac Coherent Light Source (LCLS-II) at exactly the same space and time scales, but also provide fundamental understanding of their structural transition pathways and electronic origins, which is critical for the advancement of emerging ultrafast materials science.

Type: New
Title: "Wave Dynamics in Rotating Detonation Engines using Machine-learning based Scalable Solver"

Principal Investigator: Venkat Raman, University of Michigan
Co-Investigators: Venkat Tangirala, GE Global Research
Sarah Monahan, GE Global Research
Keith McManus, GE Global Research
Peter Strakey, National Energy Technology Laboratory
Donald Ferguson, National Energy Technology Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (235,000 Summit node-hours)

Research Summary: Rotating detonation engines (RDEs) employ continuous detonation around an annulus as the mode of combustion. This feature can overcome efficiency limits of conventional gas turbines by reducing entropy increase and raising pressure within the combustor that could be used to extract useful work. Over the past decade, practical designs are beginning to emerge, which predominantly use non-premixed feed streams, implying that fuel and oxidizer enter the detonation chamber continuously and separately. The combustion process itself is then controlled by turbulent mixing ahead of the arrival of the detonation wave. An important metric for design is the number of detonation waves that are sustained within the combustor at a given operating condition. Currently, there exist only empirical correlations to predict the number of waves.

The purpose of this work is to understand the physics of wave formation through highly-resolved computations. In particular, a set of transient simulations with variable inflow conditions is used to induce transition in wave structure, thereby understanding the detonation formation mechanism. Such simulations involve not just spatial complexity in the form of very high degrees of freedom (> 109), but also require long-time temporal integration in order to capture the transition process. In order to optimally reach such length and time scales, compressible flow solvers are recast as machine learning based kernels on GPUs. This approach efficiently uses GPUs, with many operations only limited by communication bandwidth. If successful, these simulations will produce the first high-resolution insight into the formation of waves in RDEs. This information will directly aid the design of RDEs with predictable heat transfer characteristics.