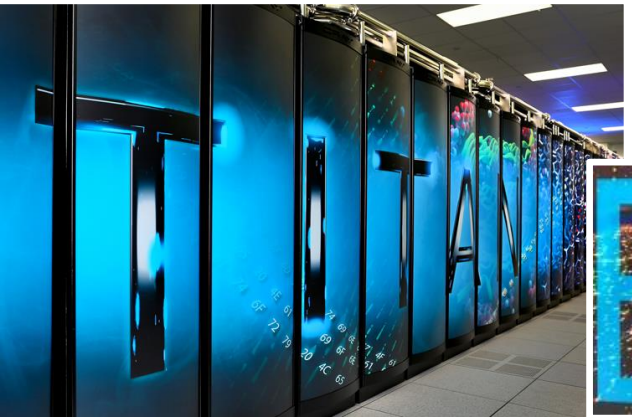
U.S. DEPARTMENT OF ENERGY | Office of Science

ASCR Leadership Computing Challenge

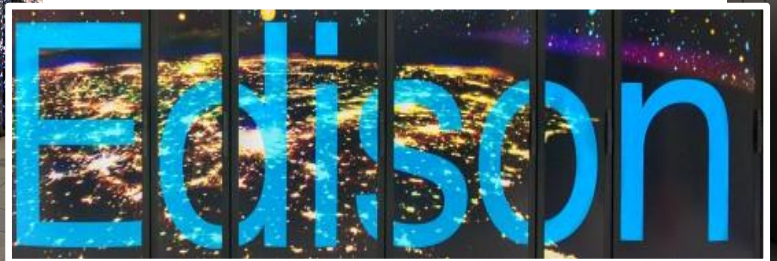
2014-2015 ALCC Project Highlights

OAK RIDGE National Laboratory

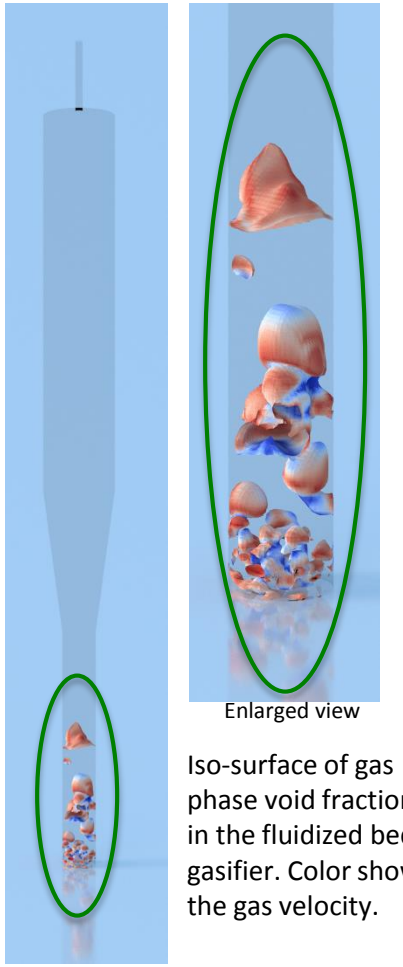
Argonne NATIONAL LABORATORY



BERKELEY LAB Lawrence Berkeley National Laboratory



Uncertainty Quantification For Reactive Multiphase Flow Simulations in Coal Gasifiers



Enlarged view

Iso-surface of gas phase void fraction in the fluidized bed gasifier. Color shows the gas velocity.

Scientific Achievement

In a fluidized bed gasifier, the H_20 to O_2 ratio plays a dominant role in the production of H_2 and CO. Conversion between H_2 and CO is captured through an ash catalyzed, water-gas shift reaction.

Significance and Impact

First-of-its-kind study using forward propagation of uncertainties in key design variables and operating factors for a fluidized bed gasifier. Adequate assessment of input uncertainties is essential in simulation driven reactor design.

Research Details

- Non-intrusive, Bayesian uncertainty quantification techniques were employed to investigate the effect of various reaction models and hydrodynamics in simulations of a fluidized bed coal gasifier.
- Sampling simulations for transient 3D reacting multiphase flow were performed for forty-five different cases with MFIX[1].
- Segregation of solids (coal and sand) in the fluidized bed adversely effects the hydrodynamics and the kinetic models.
- Use of catalytic water-gas shift is key in maintaining the proper H_2 to CO ratio.

PI: Aytekin Gel, NETL

[1] https://mfix.netl.doe.gov

Simulations were performed at NERSC.

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National Energy Technology Laboratory
ALPEMI CONSULTING
imagination at work

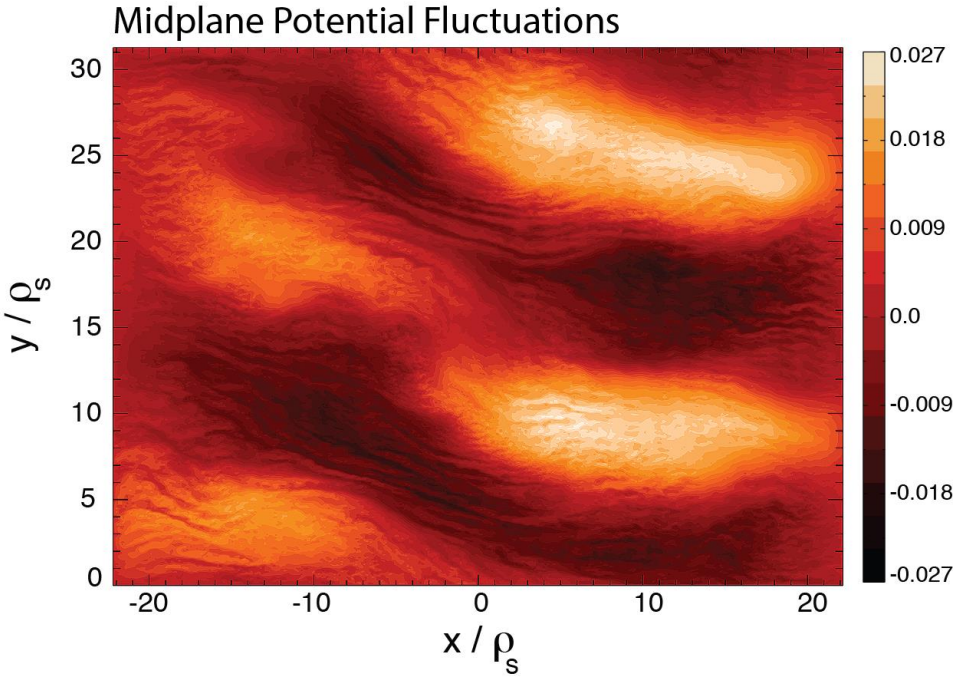
Multiscale Simulations Yield New Insights into Tokamak Turbulence

Scientific Achievement

Gyrokinetic simulations discovered new multiscale interactions that yield improved predictions of tokamak transport and confinement

Significance and Impact

The simulations show how long and short wavelength turbulence interact and nonlinearly couple in tokamaks, improving our predictive capabilities for both current and future experiments such as ITER



Snapshot of predicted midplane fluctuations in the Alcator C-Mod tokamak

Research Details

- Used GYRO code to perform nonlinear, initial value multiscale gyrokinetic simulations of Alcator C-Mod which incorporated both ion and electron gyroradius-scale turbulence at realistic ion-electron mass ratio
- These multiscale simulations matched experimental observations while separate ion or electron-scale simulations did not

N. T. Howard, C. Holland, A. E. White, M. Greenwald, and J. Candy, Nucl. Fusion **50**, 014004 (2016)

U.S. DEPARTMENT OF ENERGY | Office of Science | FES

PI: C. Holland (UCSD)
50M Hours

Chombo-Crunch: Pore Scale Reactive Transport Processes Associated with Carbon Sequestration

Scientific Achievement

First ever simulations of resolved flow and reactive transport in fractured subsurface materials

Significance and Impact

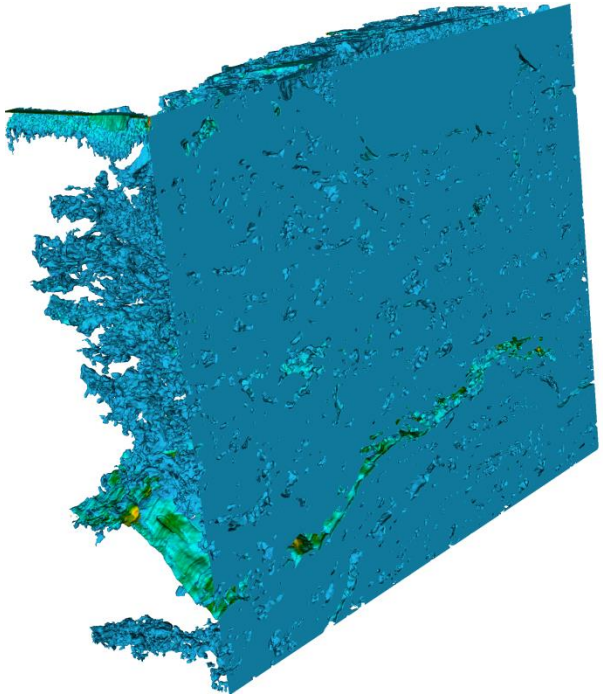
The ability to simulate resolved flow in shales will help geoscientists better predict caprock integrity for storing CO_2 as well as understanding the effects of hydrofracturing.

Research Details

- The high performance production simulation code Chombo-Crunch, developed as part of EFRC-NCGC, solves flow and reactive transport in complex geometries
- An adaptive finite volume method is used to resolve flow and transport processes at very fine scales in pore-scale geometries obtained from image data of real subsurface rocks that exhibit tight pore spaces and fracture apertures.

• NERSC Resources Used

- Edison/Hopper: ~100,000,000 raw hours used
- Archival storage: 723 TB, Project storage: 4 TB



Simulation of resolved flow in Marcellus shale. Projected surface plot of velocity shown. Simulation performed on 60,000 cores NERSC Hopper. Data in based upon FIB-SEM imagery obtained by Lisa Chan at Tescan USA and processed by Terry Ligocki (LBNL), courtesy of Tim Kneafsey (LBNL)

Trebotich and Graves, *CAMCoS*, 2015
Trebotich et al. *CiSE*, 2014
Molins et al., *ES&T*, 2014

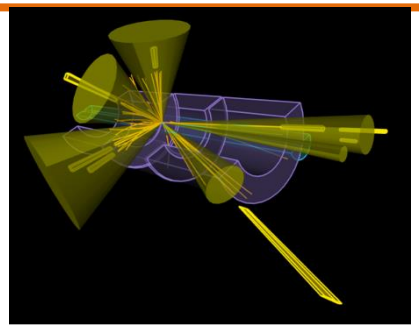
Simulation of Large Hadron Collider Events

Impact and Approach

- The ATLAS experiment at the Large Hadron Collider relies on comparison between simulated and reconstructed events. Generating these events on Mira has advanced the time to science by 12-18 months.
- We take single-threaded tasks, run them as separate MPI ranks, with an initial step of coordinating input parameters, and a final step of aggregating the output.
- ATLAS' overall needs are roughly 1 billion x86-hours per year. This award covered 6% of a year's worth of computing. If we were a country, we would be the 7th largest. This only "fits" in capability partitions.

Accomplishments

- Details of the scientific impact will need to wait until the data is collected (0.1% is on tape so far) but 49% of ATLAS papers from the previous detector period used the equivalent data set.
- We were able to generate events that were too complex for our standard production.



An example of an LHC proton-proton collision event simulated at NERSC. This event produced two electrons (yellow) accompanied by several jets of particles (green).

At NERSC

- We used 2M hours at NERSC for development, testing, debugging and urgent production. Having two different architectures (NERSC and ALCF) helped us zero in on problems by comparing performance.
- The long run queues were helpful in isolating the causes of scaling difficulties; the NERSC allocation was critical to the overall success.
- This award allowed us to develop, test and scale our code in order to make a successful application for NERSC time in the 2015 ALCC cycle, where we received 16M hours.
- Under that award, we have integrated NERSC into the ATLAS production system .

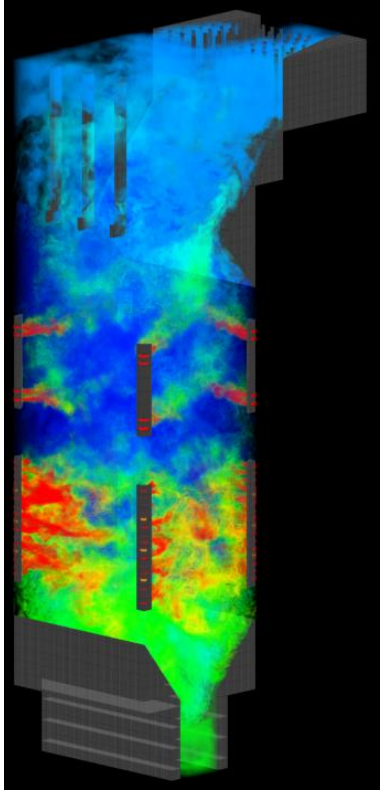
PI: T. LeCompte

Large Scale Turbulent Clean Coal Combustion

2014-2015 ALCC Project
PI: Martin Berzins, Univ. of Utah
Allocation: 30M hours
Usage: 29M hours

Science Objectives

- Further improve Uintah's modeling capability to guide the design of next-generation oxy-coal boilers for clean energy.
- Continue to develop Reverse Monte Carlo Ray Tracing (RMCRT) for modeling radiative heat transfer, implementing and testing the algorithm at large scale on both CPUs and GPUs.
- Examine the scaling and performance of the Hypre linear solver package at large core counts, utilizing the multi-threaded solver capabilities on-node.



Large Eddy Simulation of the oxy-coal combustion process in the Boiler Simulation Facility. A volume rendering of the Oxygen concentration is shown.

OLCF Contribution

- Development effort utilized a large percentage of Titan's cores and GPUs.
- User Support team was prompt and knowledgeable.
- Titan is well administered with most major third party libraries pre-compiled.
- Good online resources with details on compiling, running and debugging.

Science Accomplishments and Impact

- Demonstrated good strong scaling of the multi-level RMCRT algorithm on 262,000 CPUs and 4,096 GPUs on Titan.
- Work supports code development for enabling full-machine utilization (CPU and GPU) of the largest possible Large Eddy Simulations for oxy-coal boiler modeling.

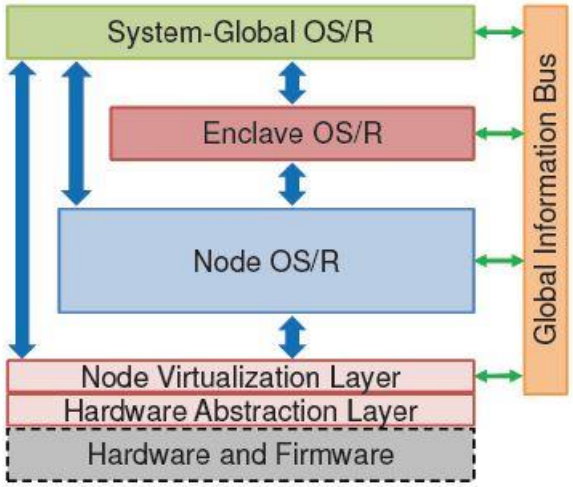
A. Humphrey, T. Harman, M. Berzins and P. Smith. "A Scalable Algorithm for Radiative Heat Transfer Using Reverse Monte Carlo Ray Tracing". *The International Supercomputing Conference (ISC'15)*, July 12-16, 2015, Springer LNCS, Frankfurt, Germany

HOBBES: Operating System and Runtime Research for Extreme Scale

2014-2015 ALCC Project
PI: Ron Brightwell, Sandia
Allocation: 30M
Usage: 27M

Science Objectives

- Provide a system software environment that enables application composition through lightweight virtualization, a model that provides needed flexibility for extreme-scale systems.
- Evaluate operating system and runtime (OS/R) interfaces and mechanisms at scale—a critical exercise to meet the challenges facing extreme-scale systems in the next five years.



Schematic representation of the main components of the Hobbes architecture and their interactions via APIs (vertical arrows) and data exchange (horizontal arrows).

Science Accomplishments and Impact

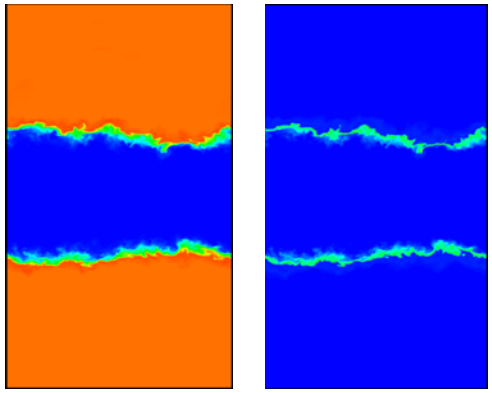
- Carried out initial testing of enclave and composition on Cray platforms.
- Developed techniques and a Palacios-based toolchain for VMM-based injection of code into an uncooperative guest. Such “guarded modules” allow the VMM to safely extend itself (and its privileged access to hardware) into the guest. (Code included in Palacios).
- Designed and implemented emulation of Intel hardware transaction memory within a VMM. The technique described avoids instruction emulation and requires only minimal instruction decoding.
- Extended Palacios VMM codebase to support memory reference tracking, VMM-internal DVFS control, and VMM-internal swapping/pinning (code included in Palacios).

High-Fidelity Simulations of Combustion Approaches with Increased Efficiency and Reduced Emissions

2014-2015 ALCC
PI: Peter Cocks
UTRC
Total Allocation: 20M hours
Total Usage: 18M hours

Science Objectives and Impact

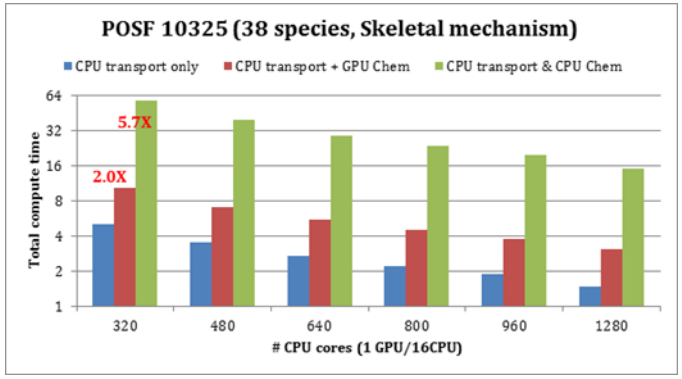
- Gain a better understanding of the phyiscal processes occurring in a rotating detonation engine (RDE).
- Demonstrate feasibility and speed-up benefits of using hybrid CPU-GPU computing in turbulent combustion simulations that employ detailed chemical kinetics for realistic alternative jet fuels for aviation.
- This work highlights the predictive capabilities of computational fluid dynamics for RDE physics.
- Enables higher-fidelity turbulent combustion calculations in aero-engine combustors to predict pollutant emissions accurately.



Snapshot images from simulation of periodic turbulent reacting jet (flow left to right). Transport part of the Navier-Stokes equations solved with CPUs and chemistry parts solved with GPUs.

OLCF Contribution

- Using Titan's hybrid CPU-GPU architecture, the team achieved a 6x speedup compared to CPU-only simulations for realistic jet fuels.



Science Accomplishments

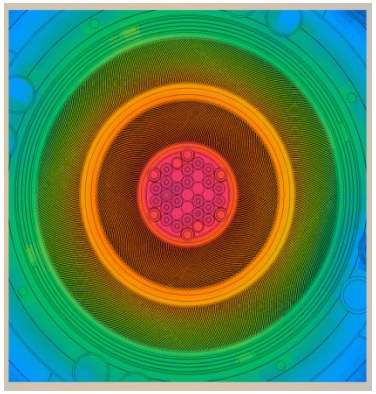
- Heat release outside of detonation front found to impact wave speed.
- Demonstrated six-fold speedup of overall computational fluid dynamics while using realistic aviation fuel kinetics in a hybrid CPU-GPU approach.
- Further speed improvements are possible by hardware improvements or other software optimizations.

Advanced Simulation of HFIR for LEU Conversion

2014-2015 ALCC
PI: Gregory Davidson , ORNL
Total Allocation: 50,000,000
Total Usage: 46,061,538

Science Objectives

- Demonstrate scaling of Shift depletion capabilities to leadership class computing platforms.
- Calculate HFIR reactivity coefficient and fuel concentrations through a complete fuel cycle.
- Examine the use of Shift depletion on target analysis.



Neutron flux in a detailed simulation of the HFIR core

OLCF Contribution

- OLCF hardware (specifically Titan) has enabled us to study the scaling of Shift to large core counts.
- OLCF hardware has enabled unprecedented turnaround time on HFIR depletion results.

Science Accomplishment and Impact

- Complete scaling study of Shift's MSOD parallelism algorithm on leadership-class hardware.
- Depletion benchmarks show good agreement with the Serpent Monte Carlo-depletion code, but some difference with VESTA.
- Improved Shift scaling results in a factor of 38 reduction in wall time compared to VESTA.
- Initial target activation results are promising and motivating a further refinement in flux group structure.

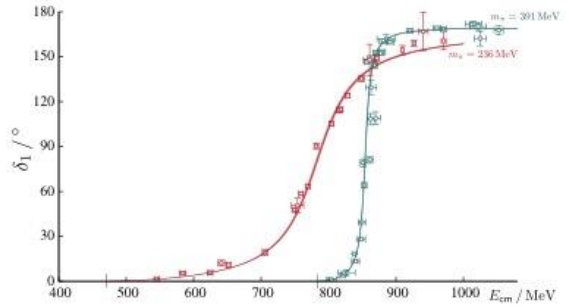
Pandya, et al., "Implementation, Capabilities, and Benchmarking of Shift, a Massively Parallel Monte Carlo Radiation Transport Code." *Journal of Computational Physics* (2015).

The Spectrum and Properties of Exotic Mesons in Quantum Chromodynamics

2014-2015 ALCC
PI: Robert Edwards, Jefferson Lab
Total Allocation: 250,000,000
Total Usage: 349,045,569

Science Objectives

- Determine the existence of "exotic" mesons from Quantum Chromodynamics theory of the strong nuclear force.
- Determine scattering amplitudes of sub-atomic particles, and resonance properties, to guide experimental searches in the new GlueX experiment at Jefferson Lab.
- Aim to predict the masses of exotic meson states in advance of the first experimental results of GlueX.



Results show the Isospin 1 P-wave scattering phase shift computed at two pion masses. Results to be submitted to Phys. Rev. D.

OLCF Contribution

- OLCF support staff contributed to making Rhea available for construction of quark sources.
- Large computing resource made available by Titan for computing large numbers of quark propagators – the solution of the Dirac equation – that feature in construction of Euclidean correlation functions.

Science Accomplishment and Impact

- First demonstration of coupled-channel scattering directly from QCD.
- Determined the resonance properties and couplings to decay products.
- Constructed annihilation quark propagators that will be used in further calculations of scattering amplitudes.
- Demonstrated efficacy of finite-volume techniques for determining amplitudes of possible exotic mesons in QCD and finding their decay modes.

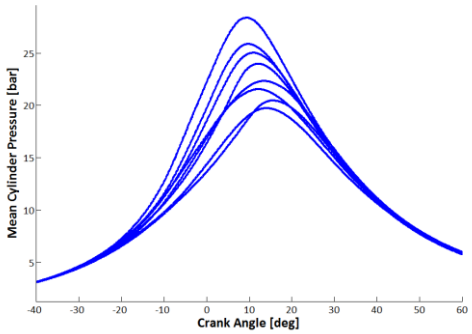
Dudek, Jozef J., Robert G. Edwards, Christopher E. Thomas, and David J. Wilson. "Resonances in Coupled π K − η K Scattering from Quantum Chromodynamics." *Phys. Rev. Lett.* 113.18 (2014).

Simulating Cyclic Variability in Dilute Internal Combustion Engine Operation

2014-2015 ALCC
PI: Charles Finney, ORNL
Total Allocation: 17,500,000 hours
Total Usage: 18,044,673 hours

Science Objectives

- Use advanced simulation techniques to understand the cyclic variations of combustion in engines.
- Understand dilute combustion instabilities to help accelerate implementation of new engines designed to meet improved fuel economy goals.
- Working to help get fuel efficiency standards in line with increasingly stringent fuel-economy and emissions standards.



Cylinder pressure during the combustion phase for different engine cycles showing dispersion under parametric variation. Mapping the range and nature of cyclic dispersion of a wide parameter space helps understand the nature of factors contributing to cyclic variability.

OLCF Contribution

- Project began using a Director's Discretionary allocation to scale and debug code.
- Team made extensive use of user support documentation and project management tools.
- OLCF resources allowed more rapid turnaround and enabled large-scale parametric studies that would otherwise not be reasonably practicable.

Science Accomplishment and Impact

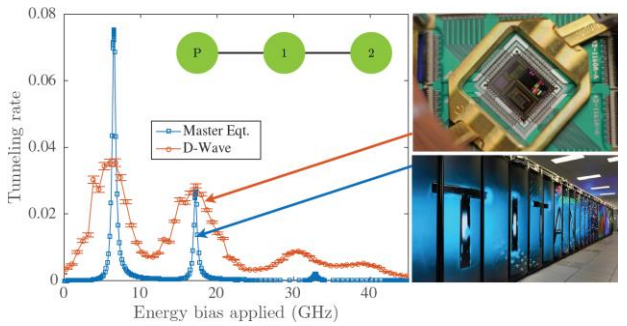
- Team identified parametric sensitivities factoring into higher cyclic variability and identified potential feedback mechanisms from one cycle to the next.
- As a result of ensemble simulations, the team was able to see the sensitivity of combustion output metrics change the parametric input values, allowing the team to rank these figures by importance.
- These results achieved the project milestone of producing a single-pass metamodel.

Quantum Computational Science

2014-2015 ALCC
PI: Itay Hen,
University of Southern California
Total Allocation: 45,000,000
Total Usage: 39,749,640

Science Objectives

- Characterizing and the uncovering of the physics driving the experimental D-Wave Two chip, a quantum annealing (QA) optimizer.
- Benchmarking of the D-Wave Two chip, in order to isolate potential "quantum enhancements."
- Finding practical applications for currently-available and near-future QA devices.
- Offering better designs for future QA chips.



Tunneling rate for the three qubit problem (shown in the inset) calculated using the quantum adiabatic master equation (run on Titan) compared against the D-Wave experimental results in Lanting et al., PRX 4, 021041 (2014).

OLCF Contribution

- The vast computing resources gave us the unique opportunity to simulate quantum computers of sizes that come close to current prototypical experimental devices, allowing us to tap into the complex structure of quantum dynamics of many-body systems in ways that so far have been considered prohibitive.
- OLCF staff provided prompt assistance in setting up more advanced simulations.

Science Accomplishments

- Creation of efficient algorithms to find *all* minimizing configurations of classically-hard optimization problems. Immediate practical applications are software V&V and circuit fault-detection.
- Successful modeling of the physical mechanism driving the experimental D-Wave chip, a quantum annealing-based optimizing device (see figure).
- Finding suitable benchmarks for experimental quantum annealers.
- Simulating optimal adaptive protocols for quantum state estimation.

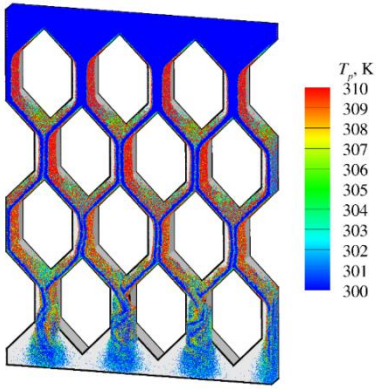
Albash, et al., "Consistency Tests of Classical and Quantum Models for a Quantum Annealer." *Physical Review A* (2015).

Simulating Multiphase Heat Transfer in a Novel Receiver for Concentrating Solar Power Plants

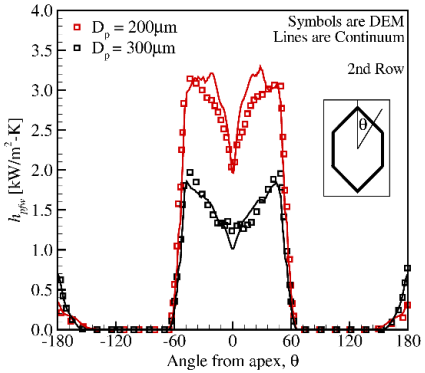
2014-2015 ALCC
PI: Christine Hrenya
University of Colorado, Boulder
Total Allocation: 15,000,000
Total Usage: 10,563,498

Science Objectives

- Develop and validate a first principles continuum model that can accurately predict the heat transfer to flowing particles.
- Assess the validity of the model by comparisons to discrete element simulations of a laboratory scale receiver.
- Better understand how the heat transfer depends on receiver configuration and aid in design.



DEM simulations of 300 micron particles colored by temperature



DEM and continuum (new model) comparisons of local heat transfer coefficient

OLCF Contribution

- These simulations are the largest MFIX-DEM simulations to date and require OLCF resources.
- The OLCF support team has promptly and efficiently addressed all of team's problems and helped us best use the computing facilities.

Science Accomplishment and Impact

- Team developed a Nusselt number correlation for the heat transfer boundary condition using DEM simulations. Unlike previous models, the new continuum model is valid for dilute to dense flow regimes and incorporates particle size effects. Further the new model is fundamentally derived and does not contain empirical parameters.
- The new continuum model closely matches DEM data (local and integrated heat transfer).
- The continuum model accurately matched DEM heat transfer data for different geometric configurations, flow rates, and particle sizes.

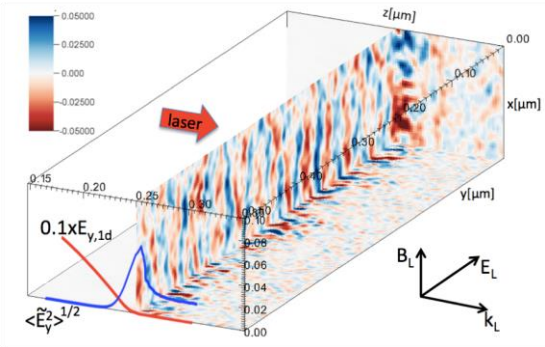
Morris, et al., "A Conductive Heat Transfer Model for Particle Flows over Immersed Surfaces." *International Journal of Heat and Mass Transfer* (2015).

Laser-Driven Relativistic Electron Beam Filamentation in Solids

2014-2015 ALCC
PI: Andreas Kemp
LLNL
Total Allocation: 30M hours
Total Usage: 19M hours

Science Objectives and Impact

- Use state-of-the-art particle kinetic particle simulations to characterize conditions found in solid-density plasma during the interaction with sub-100fs laser pulses.
- Study absorption of sub-100fs laser pulses on solid density targets.
- Transition between absorption- and electron transport regions, i.e. the surface of a solid target.



Field fluctuations [Ey − Ey,1d] due to plasma waves in a highly resolved 3D PIC simulation, shown near the target surface at z = 0.25μm. Laser is incident from z = 0.

OLCF Contribution

- User support was instrumental in helping get team's MPI code to run at scale on Titan.
- Website was helpful in determining resources up and down time, as well as availability.

Science Accomplishments

- Successfully simulated the interaction of intense sub-100 femtosecond laser pulses in one, two, and three dimensions.
- One-dimensional modelling showed researchers that they needed to resolve electron skin depth.
- Team isolated physics effects that lead to target heating.

Calculation of Neutron Scattering Cross Section of Plutonium and its Compounds

2014-2015 ALCC
PI: Gabriel Kotlier, Rutgers Univ
Allocation: 90,000,000
Usage: 96,182,232

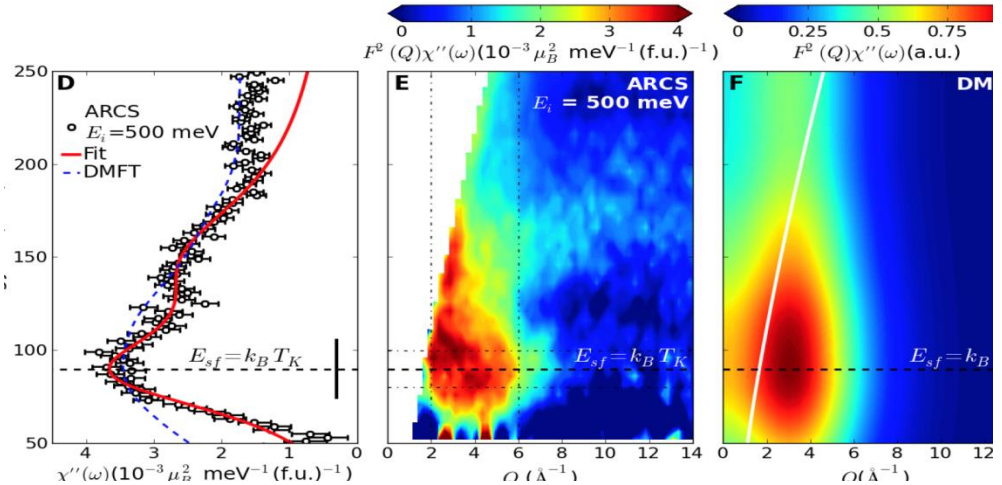
Science Objectives

- Identify plutonium's "missing" magnetism.
- Predict spin dynamics and electron excitations in plutonium's delta phase using a combination of density functional theory (DFT) calculations and the leading-edge dynamical mean field theory (DMFT) technique.

OLCF Contributions

- Over 40M core hours available on Titan were essential for our simulations. These resources are unique in the world.
- Support from OLCF is outstanding. Problems are typically resolved within hours.

Marc Janoschek, et al. "The Valence-Fluctuating Ground State of Plutonium," *Science Advances* **1**, no. 6 (2015): e1500188. doi:10.1126/sciadv.1500188



Comparison of the predicted S(q,ω) for δ-Pu (right) with the experimental observations (middle). Left panel shows the q integrated intensity in absolute units with statistical errors shown. Larger systematic error bars in the experimental data at low and high energy are not shown.

Science Accomplishment and Impact

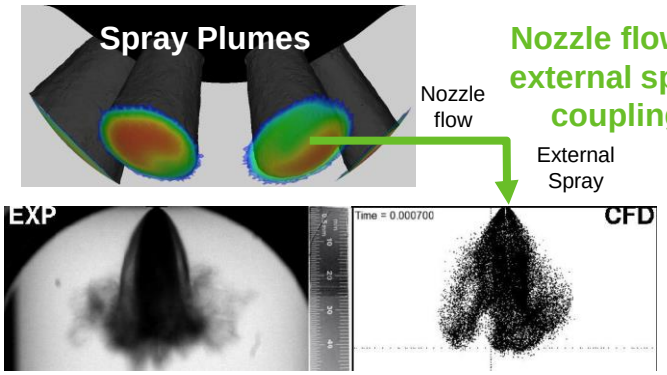
- Developed an algorithm to predict the electronic free energy of solids implementing DFT+DMFT.
- Used Titan to predict neutron excitations as a function of energy and momenta, and compared the results with neutron scattering via ORNL's SNS.
- Revealed the ground state of plutonium is governed by valence fluctuations — a quantum-mechanical superposition of localized and itinerant electronic configurations.
- Results resolve the long-standing controversy between experiment and theory on plutonium's magnetism.
- Suggest an improved understanding of the effects of such electronic dichotomy in complex materials.

Multi-Hole Injector Optimization for Spark-Ignited Direct-Injection Gas Engines

2014-2015 ALCC Project
PI: Tang-Wei Kuo, GM
Allocation: 15,000,000
Usage: 10,883

Science Objectives

- Reduce the design time of future combustion systems concepts.
- Develop a procedure to couple Eulerian nozzle internal flow computations as initial conditions to external Lagrangian spray simulations.
- Compare simulation results to experimental optical spray vessel measurements over 35 thermodynamic conditions spanning flash boiling.



Internal nozzle flow computations are used to initialize external spray calculations. The procedure is validated against experiments.

OLCF Contribution

- Wael Elwasif developed an automated framework to submit and manage a large number of ensemble simulations.
- OLCF help desk provided top-notch customer service on data management and software tools.
- OLCF User Meeting proved valuable for face-to-face project reviews and networking with the wider HPC community.

Science Accomplishments and Impact

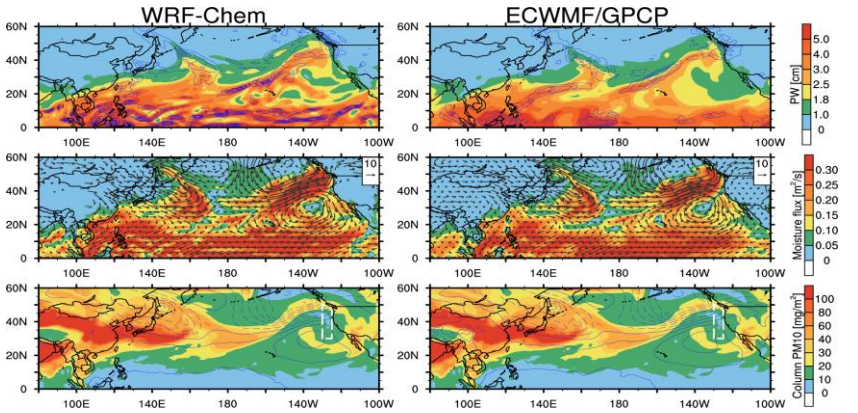
- The model successfully captures the regime transition of the spray.
- Flare flashing leads to spray collapse due to interaction of widening spray plumes.
- The analytical methodology shows promise to predict spray shape and streamline the injector selection process.

Multi-scale Water Cycle Processes in Climate Change: Sensitivity to Modeling Frameworks

2014-2015 ALCC Project
PI: Ruby Leung, PNNL
Allocation: 18,000,000
Usage: 20,227,132

Science Objectives

- Test and evaluate a non-hydrostatic global variable resolution modeling framework for climate simulations.
- Evaluate the sensitivity of simulated atmospheric river frequency to model resolution.
- Understand the role of long-range dust transport associated with North Pacific atmospheric rivers.



Atmospheric moisture and long-range transported dust associated with an atmospheric river on January 24, 2012 simulated by the model (left) and from observations (right**).**

OLCF Contribution

- High resolution MPAS-A simulations and WRF-Chem simulations require massively parallel computing platforms for reasonable throughput and mass storage to archive the large volume of model outputs for analysis.

Science Accomplishments and Impact

- The non-hydrostatic Model for Prediction Across Scales (MPAS) coupled to CAM5 physics has been ported to Titan for idealized aquaplanet and real world AMIP simulations.
- Analysis indicated lower sensitivity of non-hydrostatic MPAS-CAM5 simulations to model resolution compared to previous simulations using the hydrostatic MPAS-CAM4 model.
- WRF-Chem simulations used to quantify the contributions of long-range transported dust to total aerosol mass along the U.S. west coast during atmospheric river landfall.

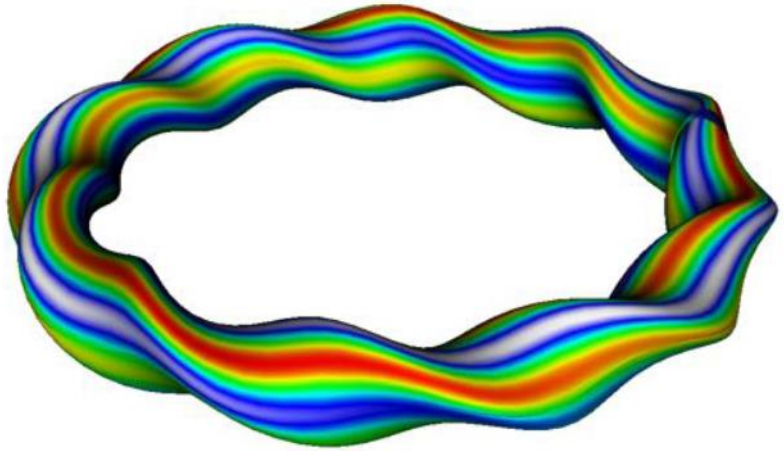
Kim, Zhou, Gao, Fu, Johnson, Huang, and Liu. "Spatially Resolved Estimation of Ozone-related Mortality in the United States under Two Representative Concentration Pathways (RCPs) and Their Uncertainty." *Climatic Change* (2014).

Gyrokinetic Simulation of Energetic Particle Turbulence and Transport

2014-2015 ALCC Project
PI: Zhihong Lin, UC Irvine
Allocation: 50,000,000
Usage: 110,992,826

Science Objectives

- Build a predictive capability for energetic particle turbulence and transport in burning plasmas in support of ITER.
- Accurately predict confinement properties of energetic particles produced by fusion, incorporating kinetic effects, nonlinear interactions, Alfven eigenmodes, cross-scale couplings of microturbulence, and shear Alfven wave turbulence.



GTC simulation of Alfven eigenmode structures In LHD. [Spong, 14th IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, 2014, Vienna]

OLCF Contribution

- Helped port GTC gyrokinetic particle code to Titan and optimize GTC for the GPUs.
- Assisted large-scale GTC simulation to resolve kinetic effects in the magnetohydrodynamic instability (Alfven eigenmode).

Science Accomplishments and Impact

- New simulation capability addresses 3-D symmetry-breaking effects on fast-ion instabilities and turbulence in toroidal fusion systems.
- Prediction of energetic particle confinements in ITER burning plasmas.
- Nonlinear generation of zonal fields by Alfven eigenmode.
- Critical-gradient model for energetic particle transport.

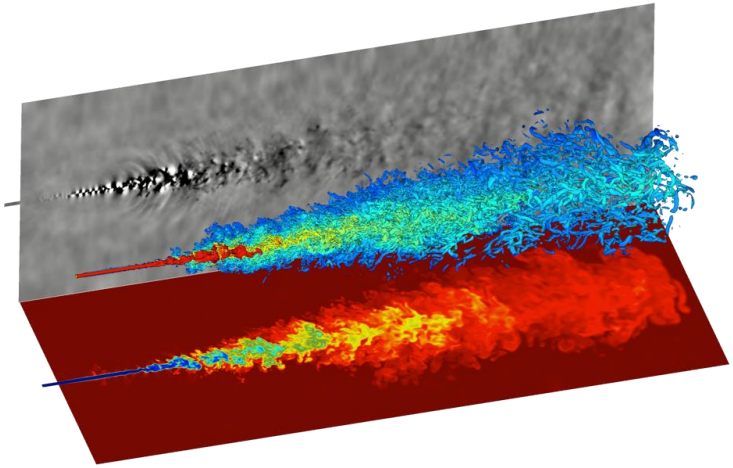
Wang, Zhixuan, Zhihong Lin, Wenjun Deng, Ihor Holod, W. W. Heidbrink, Y. Xiao, H. Zhang, W. Zhang, and M. Van Zeeland. "Properties of Toroidal Alfvén Eigenmode in DIII-D Plasma." *Physics of Plasmas* 22.2 (2015)

Development of Multiphase Combustion Models for LES of Advanced Engine Systems

2014-2015 ALCC Project
PI: Joseph Oefelein, Sandia
Allocation: 75,000,000
Usage: 77,664,329

Science Objectives

- Perform fundamental inquiries into the structure and dynamics of turbulent combustion processes that are dominated by high-pressure, high Reynolds number, multiphase flows in advanced engine systems.
- Directly couple Large Eddy Simulation (LES) to corresponding experiments being performed in High Pressure Combustion Facility and Turbulent Combustion Laboratory at Sandia.



Three-dimensional rendering of supercritical fuel injection processes at Diesel engine conditions (n-dodecane – air, 60 bar). Axial velocity (center), pressure (back), temperature distribution (bottom).

OLCF Contribution

- Ramanan Sankaran collaborated with team to refactor the RAPTOR code framework to hybrid MPI/OpenMP/OpenACC framework.
- OLCF enabled in-situ data processing and visualization via the remote capabilities of Ensight and Paraview.

Science Accomplishments and Impact

- First treatment of multi-physics, multi-scale processes associated with IC-engines at actual operating conditions (e.g., Re ~ 10^6).
- Development of advanced multiphase model framework that includes detailed thermodynamics and transport associated with fuel injection at supercritical pressures (e.g., p ~ 60 bar).
- Development and validation of an advanced combustion closure coupled with optimized finite-rate chemical kinetics.

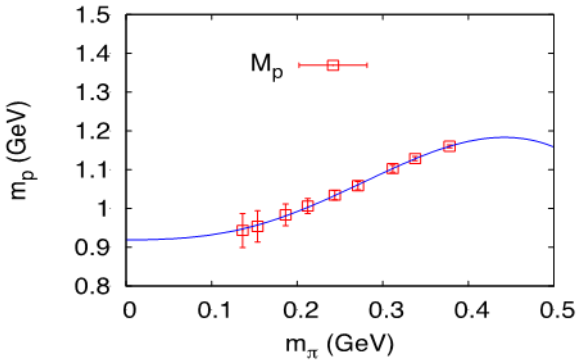
Lacaze, Guilhem, Antony Misdariis, Anthony Ruiz, and Joseph C. Oefelein. "Analysis of High-pressure Diesel Fuel Injection Processes Using LES with Real-fluid Thermodynamics and Transport." *Proceedings of the Combustion Institute* (2015)

Quark and Glue Structure of the Nucleon with Lattice QCD

2014-2015 ALCC
PI: Keh-Fei Liu,
University of Kentucky
Total Allocation: 68,800,000
Total Usage: 87,056,778

Science Objectives

- Ab initio lattice Quantum Chromodynamics calculation of quark and gluon structures of the nucleon at the physical pion point.
- Chiral behaviors of the nucleon mass, nucleon excited states and meson spectra including exotic multiquark states.
- Decomposition of the proton spin and mass into quark and glue components. Strangeness and charmness in the nucleon.



Nucleon mass as a function of the pion mass calculated with the sea quark mass at the physical point – chi QCD Collaboration

OLCF Contribution

- Hardware resources are essential for this project. Due to the large size of the program, the team required 128 to 256 nodes for a single job.
- Support staff served as liaison between software vendor and researchers for queuing system implementation for signaling jobs.

Science Accomplishment and Impact

- The chiral behavior of the nucleon mass including the physical point is obtained for the first time with chiral fermions. This allow tests of chiral perturbation theory and the extraction of low energy constant such the π-nucleon σ term for the connected insertion.
- The leptonic decay of the ρ meson is calculated at the physical pion point for the first time and it agrees with experimental result very well. This serves as a benchmark for model calculation as well as for other lattice calculations.
- The πN scattering state is clearly observed in the negative parity nucleon channel. This will have ramification on understanding the nature of Roper resonance which is the lowest radial excitation of the nucleon.

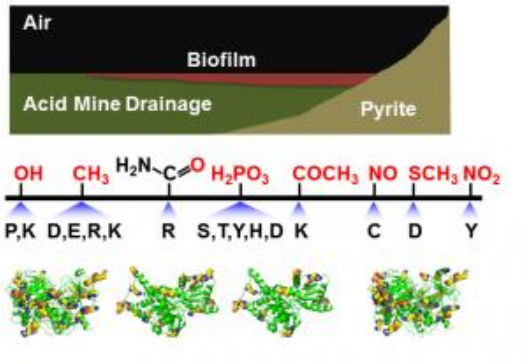
Yang, et al., "Charm and Strange Quark Masses and F D S from Overlap Fermions." *Physical Review D* (2015).

Computational Analysis of Complex Proteogenomics Data for Characterization of Terrestrial Carbon Turnover by Soil Microbial Communities

2014-2015 ALCC
PI: Chongle Pan, ORNL
Total Allocation: 25,000,000
Total Usage: 23,920,189

Science Objectives

- Characterize the carbon degradation activities of microbial communities in critical environments using metaproteomics and metagenomics.
- Elucidate the responses of microbial communities to environmental perturbations and climate changes.
- Develop and demonstrate scalable analytics of big omics data using the Titan supercomputer.



Diverse and divergent protein post-translational modifications a natural microbial community

OLCF Contribution

- We used the Titan supercomputer for large-scale data analytics from metagenomics and metaproteomics experiments. Titan's high-performance file system and interconnect allow us to compute very big datasets.
- The OLCF staff trained our postdocs to be proficient in scaling up algorithms to supercomputers and executing large computing jobs. These research experiences launched their careers as tenure-track professors.

Science Accomplishment and Impact

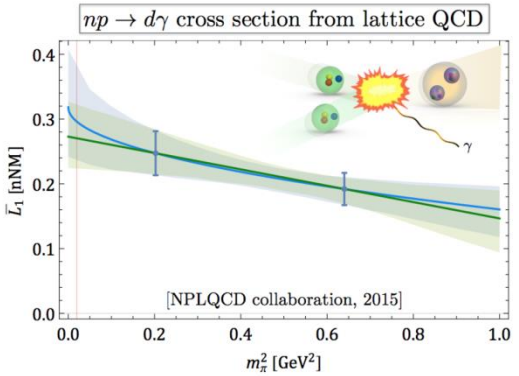
- Performed the first protein post-translational modification study of natural communities.
- Performed the first functional phylogenomics study of all sequenced prokaryotic genomes.
- Performed the first $^{15}N/^{2}H$ proteomic stable isotope probing study.
- Characterized microbial communities in many different ecosystems at unprecedented details.
- The science enabled by this project is highly relevant to BER's mission in understanding climate changes and carbon cycling.

Hypernuclei and Charmed Nuclei

2014-2015 ALCC
PI: Martin Savage,
University of Washington
Total Allocation: 65,100,000
Total Usage: 66,589,029

Science Objectives

- Determine the binding energies of hypernuclei and predict those nuclei containing a charm quark.
- Determine the spectrum of light and exotic nuclei.
- Calculate the magnetic properties of light and exotic nuclei.
- Determine the radiative-capture cross sections in simple nuclear systems.



Extrapolation of the short-distance two-nucleon interaction with a magnetic fields, calculated with Lattice QCD, to the physical pion mass. Beane et al., **arXiv:1505.02422** *(2015).*

OLCF Contribution

- Titan was used to generate ensembles of gauge-field configurations that are used to calculate nuclear correlation functions.
- Leadership-class computing resources play a critical and unique role in accurately describing the quantum mechanical fluctuations that define nuclear physics at a fundamental level.

Science Accomplishment and Impact

- The binding energy of the lightest nuclei, hypernuclei and charmed nuclei have been calculated at a pion mass of 450 MeV.
- The two-nucleon radiative-capture cross section has been determined at the physical pion mass, and found to agree with experiment. This is the first inelastic nuclear reaction to be calculated from first principles.
- The magnetic moments of light nuclei and hypernuclei have been calculated. These results indicate that the nuclear shell model is valid over a large range of light-quark masses.

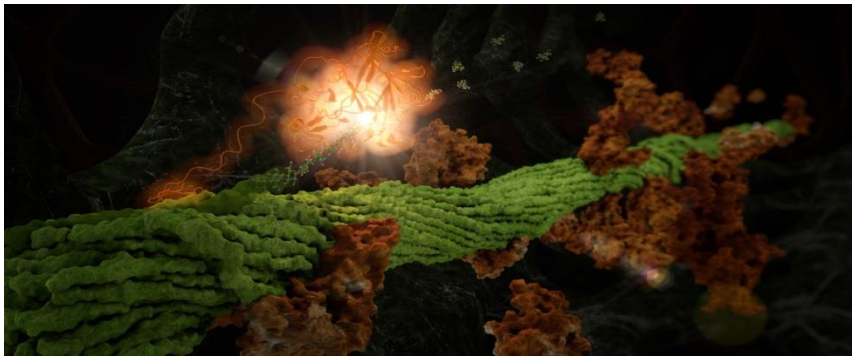
Beane, et al., "Quarkonium-nucleus Bound States from Lattice QCD." *Phys.Rev. D* (2015).

Molecular Simulation in Bioenergy

2014-2015 ALCC
PI: Jeremy Smith, ORNL and UTK
Allocation: 59,000,000
Usage: 49,422,287

Science Objectives

- Understanding the deconstruction of lignocellulosic biomass by chemical pretreatment.
- Understanding the mechanistic details of cellulase–cellulose interactions.
- The above information is crucial for the development of efficient systems for converting plant biomass to useful energy.



A cellulase enzyme (orange) hydrolyzing cellulose (green) despite the presence of lignin (brown). Image credit: scistyle.com

OLCF Contribution

- Access to OLCF resources was essential as the simulations run on ~50% of TITAN, using 9,000 nodes.
- The leadership class simulations described above produce TB of data. The OLCF Lustre and HPSS filesystems allowed for storage and analysis of the data.
- OLCF staff Suzanne Parete-Koon and Arnold Tharrington assisted with mpi issues of the GROMACS code.

Science Accomplishment and Impact

- Solvation of lignin, a major polymeric component of biomass, by tetrahydrofuran (THF) and water shifts the equilibrium structure of the biopolymer from a globular state, which poses a barrier to bioethanol production, to a coil, which allows a more efficient deconstruction of biomass to biofuels.
- Explanation of experimental work at BESC that has shown that a THF pretreatment dramatically increases the conversion of lignocellulosic biomass into biofuel.
- Obtained molecular-level structural information of cellulases while the enzymes are digesting cellulose.

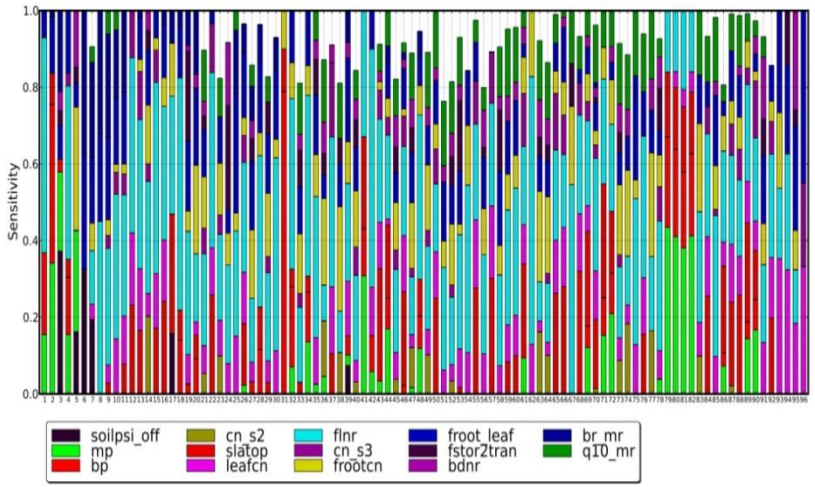
Carmona, Christopher, Paul Langan, Jeremy C. Smith, and Loukas Petridis. "Why Genetic Modification of Lignin Leads to Low-recalcitrance Biomass." *Phys. Chem. Chem. Phys.* (2015)

Delivering DOE's Next-Generation High-Resolution Earth System Model

2014-2015 ALCC Project
PI: Peter Thornton, ORNL
Allocation: 30,000,000
Usage: 33,318,336

Science Objectives

- Determine how the hydrological cycle and water resources interact with the climate system on local to global scales.
- Explore how biogeochemical cycles interact with global climate change.
- Rationalize how rapid changes in cryosphere systems interact with the climate system.



Large ensemble parameter sensitivity/ uncertainty quantification.

OLCF Contribution

- Hardware resources were essential in meeting several critical project milestones.
- User Assistance staff was very efficient in handling large number of new user account requests.
- Liaisons assisted in model optimization for best performance.

Science Accomplishments and Impact

- Explored a new approach to efficient atmospheric model evaluation, tuning, and calibration using "short ensembles."
- Developed new phosphorus-enabled biogeochemistry model, new coupled reactive-transport/biogeochemistry module, and new river routing scheme with inundation capability.
- Implemented new uncertainty quantification framework to evaluate parametric uncertainty across a large fraction of the ACME land model parameter space.

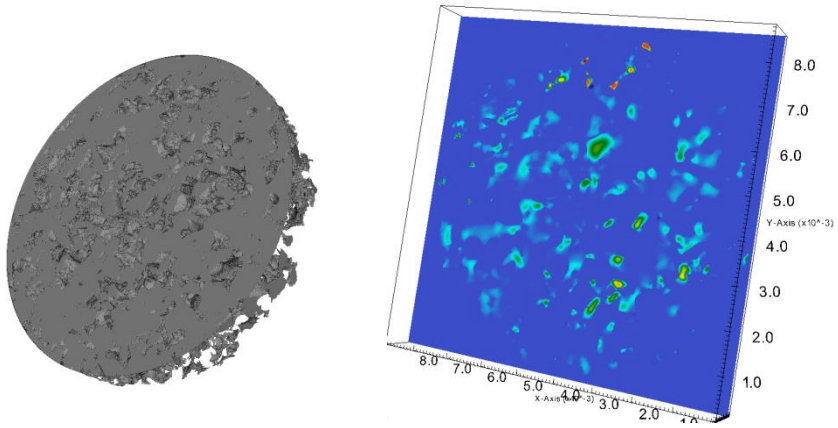
Collins et al., "The Integrated Earth System Model Version 1: Formulation and Functionality." *Geoscientific Model Development* (2015)

Chombo-Crunch: Modeling Pore Scale Reactive Transport Processes Associated with Carbon Sequestration

2014-2015 ALCC
PI: David Trebotich, LBNL
Total Allocation: 50,000,000
Total Usage: 99,977,855

Science Objectives

- Use new investigative tools to build a next-generation understanding of molecular-to-pore scale processes in fluid rock systems.
- Simulation of pore scale flow and reactive transport in a cylinder (synthetic) packed with microspheres.
- Simulation of pore scale flow and reactive transport in Bedford limestone from image micro CT image data.



Computational domain from image and steady state flow in Bedford limestone (D. Trebotich)

Application Performance

- Team's Chombo-Crunch code scales between 512 and 262,144 cores. The teams typical runs need 50-100K cores.
- Production runs for REV scale shale image data require 180,000 cores, and a Cray architecture, meaning OLCF is the facility suitable for these simulations.
- Team has seen a 15-20% improvement when using 262,144 cores.

Science Accomplishment and Impact

- Largest steady state pore scale reactive transport simulations to date (256K CPU cores, 2048x1024x1024 grid points benchmark scaling run; 128K CPU cores, 2048^3 resolution steady state production run).
- Steady state flow in Bedford limestone from image data.
- First ever simulation of resolved steady state flow in low permeability rock
- The work will lead to a better understanding of caprock integrity for subsurface carbon storage.

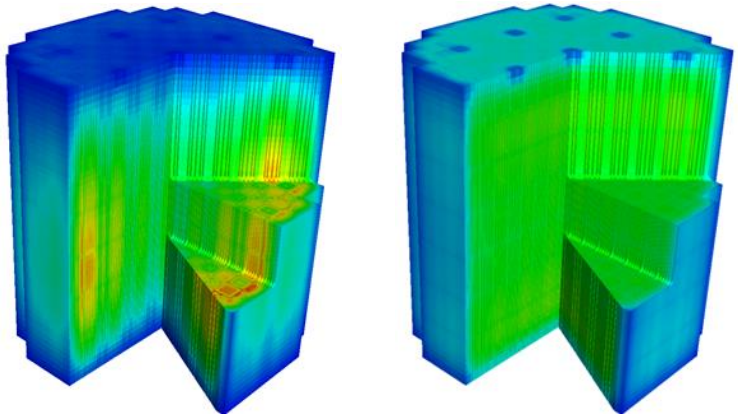
Trebotich, David, and Daniel Graves. "An Adaptive Finite Volume Method for the Incompressible Navier–Stokes Equations in Complex Geometries." *Communications in Applied Mathematics and Computational Science* (2015).

Delivering Advanced Modeling & Simulation for Nuclear Energy Applications

2014-2015 ALCC
PI: John Turner
ORNL
Total Allocation: 75,000,000 hours
Total Usage: 35,671,466 hours

Science Objectives and Impact

- Use data from pressurized water reactors (PWRs) in conjunction with high-performance computing to improve the operating efficiency, cost, and safety of nuclear power plants.
- Predict the performance of nuclear reactors by developing comprehensive, science-based simulations and models.
- Use simulation data to inform industry of best practices for safety, reliability and economics of nuclear power plants.
- Release Virtual Environment for Reactor Applications (VERA) to industry test stands.



The beginning (left) and end (right) from a simulation of 3D pin power distribution at the Watts Bar nuclear power plant.

OLCF Contribution

- OLCF staff helped the CASL team with various throughput issues on Titan that allowed them to meet its programmatic milestones.
- Supported CASL's training courses and student workshops with computing resources as well as expertise and mentoring.

Science Accomplishments

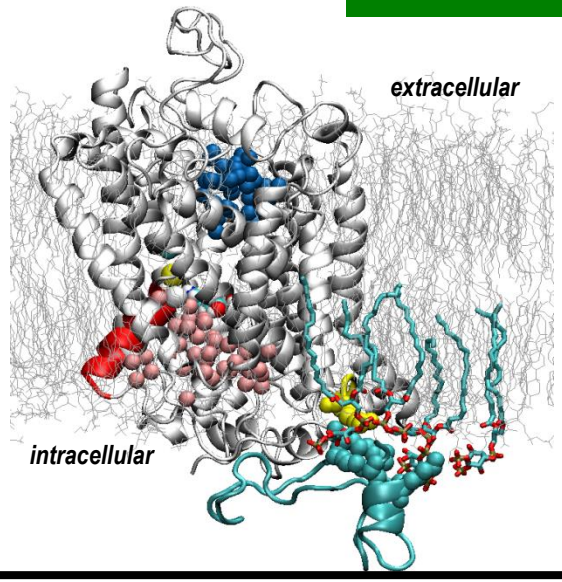
- In late 2013, team was able to large-scale coupled multi-physics model of an operating PWR. In 2014, the team was able to improve the physics model by resolving fuel rod geometry and simulations depleting reactor fuel as a function of time.
- Team was able to run significant validation testing of its physics models.

Energy Coupling in Membrane Protein Function: Mechanisms of Na^+-Coupled Transporters and Effects of their Environment

2014-2015 ALCC
PI: Harel Weinstein, Cornell
Total Allocation: 10,000,000
Total Usage: 12,005,097

Science Objectives

- To understand the functional mechanisms of the chemical energy-regulated transporter DAT in the performance of substrate translocation across membranes.
- To reveal structural and dynamic determinants of specific interactions of such transporters with charged membrane components, specifically the role of DAT/PIP_2 interactions in energy-coupled state-to-state transitions.



DAT (cartoon) in lipid membrane (sliver sticks). The association of the N-term (cyan) with intracellular (IC) loops of DAT (yellow) is mediated by PIP_2 lipids (licorice) and triggers opening of the IC vestibule of the transporter. This opening is characterized by the outward swaying of functionally relevant TM1a segment (red), water accumulation in the IC milieu (pink balls), and concomitant water depletion from the extracellular side (blue balls).

OLCF Contribution

- Having installed specialized software (ACEMD) capable of taking full advantage of the GPU architecture in the amazing resources available at OLCF, we are making otherwise impossible discoveries about molecular mechanisms.
- Expert user support received from OLCF was invaluable, especially in the initial stages.

Science Accomplishment and Impact

- Disclosed the important initial successes in determining the mode of association of the N- and C-terminal regions of the DAT protein with PIP_2 lipids, and the state-to-state transitions they trigger.
- The documented high impact of the results is due in good part to the access provided by the ALCC to the OLCF resources, which enabled the extensive simulations to reveal heretofore unidentified elements of the mechanisms of energy transfer through focused interactions between the protein, ions and specific membrane components.

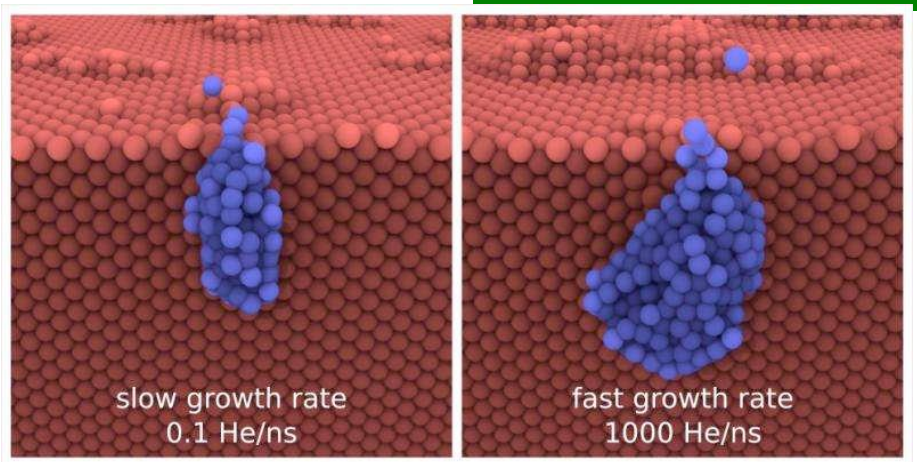
Stolzenberg et al., "Mechanism of the Association between Na Binding and Conformations at the Intracellular Gate in Neurotransmitter:Sodium Symporters." *Journal of Biological Chemistry.* (2015).

Understanding Helium Plasma Response of Tungsten Response to predict Fusion Plasma Facing Component Performance in ITER

2014-2015 ALCC
PI: Brian Wirth
University of Tennessee
Total Allocation: 30,000,000
Total Usage: 25,033,892

Science Objectives

- Realizing the promise of fusion energy requires improved knowledge of plasma-surface interactions.
- Evaluate the effect of helium gas implantation rate on tungsten surface morphology.
- Validate continuum reaction-diffusion models against atomistic simulations.



ParRep simulation of the tungsten surface morphology for helium bubbles growing inside a fusion reactor divertor.
Credit: Luis Sandoval, Arthur Voter, Blas Uberuaga, and Danny Perez

OLCF Contribution

- TITAN access used to run large-scale parallel replica dynamics simulations to evaluate He implantation rate on gas bubble growth processes.
- Evaluating GPU acceleration on TITAN, with indication of 2.3 to 4x speedup.

Science Accomplishment and Impact

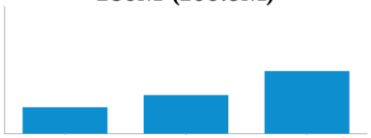
- Demonstration of ITER experimentally relevant growth rates of sub-surface He bubbles in tungsten demonstrate different surface morphology evolution and size dependence of bubble bursting with implications towards divertor performance in ITER.
- Observed that helium bubble simulations, when simulated over realistic time scales, is qualitatively different than prior traditional molecular dynamics simulations.
- Work serves as a foundation for SciDAC project attempting to create more comprehensive fusion simulations.

L. Sandoval, D. Perez, B.P. Uberuaga, A.F. Voter, "Competing kinetics and He bubble morphology in W," *Physical Review Letters* ***114,*** *105502 (2015).*

Applying Breakthroughs in Protein Structure Calculation to the Creation of Designer Enzymes

David Baker, University of Washington

ALCC 2014-2015 + INCITE 2015
280M (259.3M)



Impact and Approach

- Artificial proteins and protein-like molecules have the potential to revolutionize medicine, manufacturing, and materials science
- Advancing protein structure modeling capabilities to enable the design of novel proteins, including therapeutic peptides (as new drugs) that target diseases such as Influenza, Ebola, HIV, and Alzheimer's disease.
- Develop more accurate energy function and sample astronomical numbers of building-block sequences and molecular conformations to design a molecule with a new fold

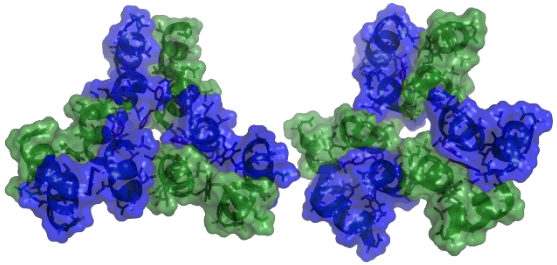
Accomplishments

- Major improvements to the physical energy model; multiple publications including the journal Structure
- Developed new multi-state design algorithms that take advantage both of the large parallel computing capacity of the Blue Gene/Q system, and the rapid cross-communication between nodes
- Designed small, folded mini-proteins (potentially useful as a new class of drugs), with the new algorithms
- Generalized conformational sampling tools to permit design of artificial heteropolymers with protein-like folds and activity

ALCF Contributions

- Helped to port & benchmark Rosetta from Blue Gene/P to Blue Gene/Q
- Helped to thread a part of the code in collaboration with IBM
- Advised on better parallelization of the code.
- Compiled the code using IBM C++ compiler

Hexameric designed artificial heteropolymer with protein-like folds but far greater *in vivo* resiliency than natural proteins.



H. Park, F. DiMaio, D. Baker; Structure. 2015 Jun 2;23(6):1123-8

Turbulent Multiphase Flows for Nuclear Reactor Safety

PI: Igor A. Bolotnov, North Carolina State university

ALCC-2014

Impact and Approach

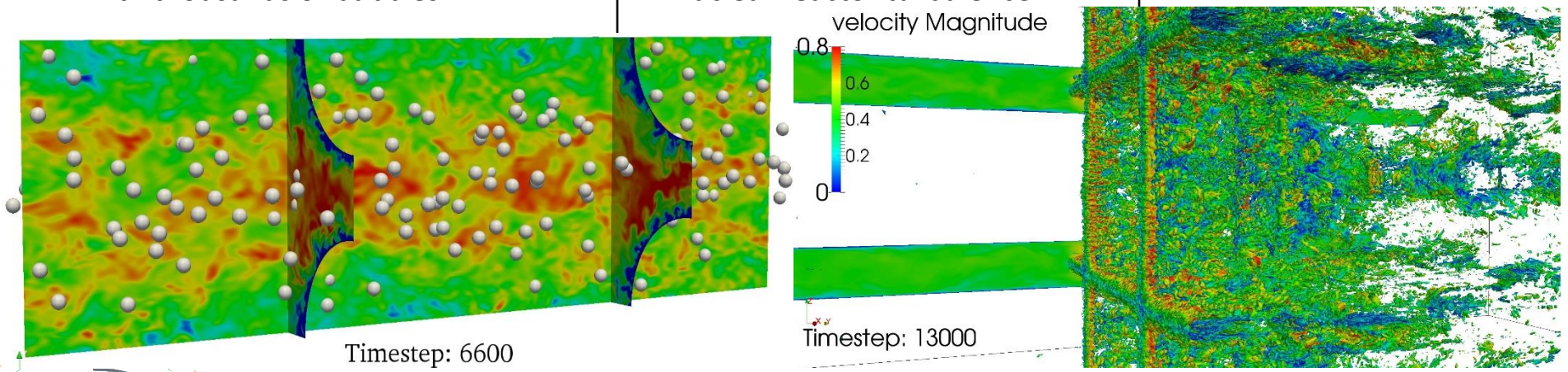
- Prediction of coolant flow behavior in nuclear reactor cores is important for reliable and safe nuclear power. It greatly benefits from virtual experiments performed using HPC.
- Fully resolved simulation of highly turbulent flows require very fine mesh resolution requiring resources available only at leadership computing facilities. Future exascale machines will allow full Reynolds number flows with thousands of bubbles.

Accomplishments

- Extensive single- and two-phase turbulence analysis has been performed for unstructured geometries and compared with previous results for simple boundary layers
- Un-precendented scale simulations created detailed bubbly turbulence datasets which will result in transformational insight into nuclear reactor turbulence.

ALCF Contributions

- Emily Shemon has been instrumental in making this project a success
- User Assistance Center, Scientific Computing Group and Visualization and Analysis Team have been very responsive and provided tremendous help during this project



Bubbly flow simulation in a nuclear reactor subchannel (1B elements with 260 bubbles, left) and reactor coolant flow through PWR core with fully resolved mixing vanes and spacer grids (2B elements at 1/10 reactor flow, right)

Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An *Ab Initio* Study of Liquid Water

PI: Robert A. DiStasio Jr. (Princeton/Cornell)

ALCC-2014
350 M

Impact and Approach

- Highly accurate benchmark atomistic simulations of liquid water and aqueous ionic solutions that are most relevant to the design of novel and clean energy materials.
- Uses state-of-the-art hybrid density functional theory (DFT) in the condensed-phase which provides an accurate *ab initio* description of exchange and correlation, including non-bonded van der Waals (vdW) forces.
- Extremely computationally demanding — only possible with algorithmic advances in conjunction with the HPC capabilities of *Mira* at ALCF.

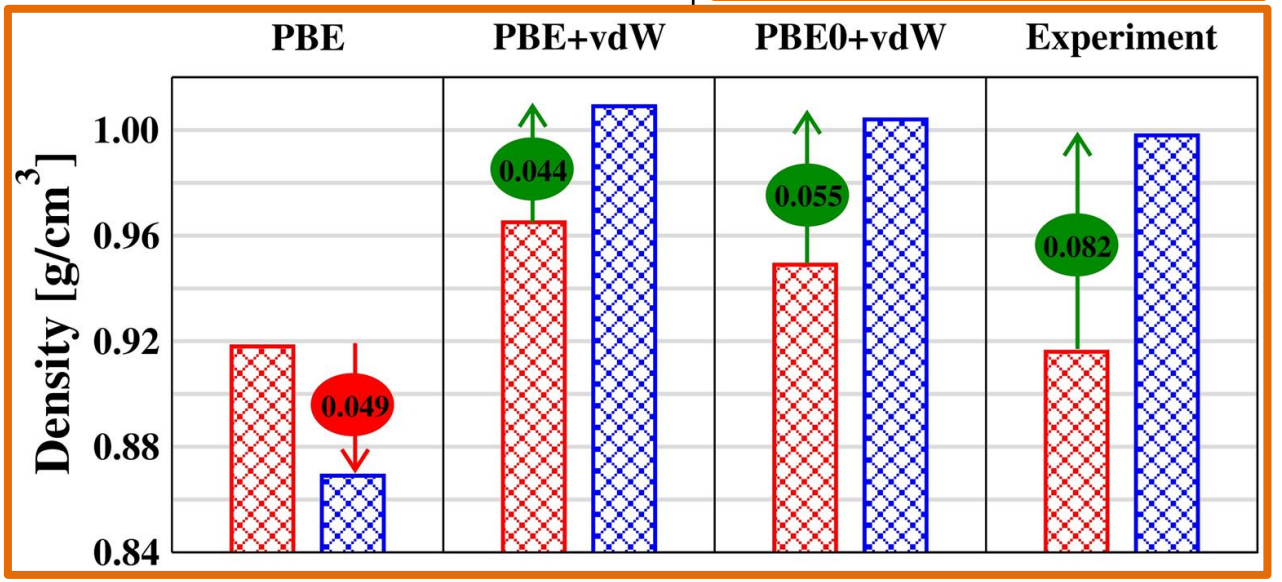
Accomplishments

- Anomalous density ordering between liquid water and ice is now accurately predicted by vdW-inclusive hybrid DFT.
- Current simulations are providing key details for a microscopic understanding of the density maximum in liquid water.
- Hydronium (H_3O^+), hydroxide (OH^-), and biologically-relevant ionic solutions also in excellent agreement with experiment.

ALCF Contributions

- With ALCF, we have developed a highly efficient Poisson solver, which significantly reduces the cost of these simulations.

*Systematic improvements in the predicted anomalous density ordering between **liquid water** and **ice** by vdW-inclusive hybrid DFT.*



Large scale quantum simulations of electrode-electrolyte interfaces

Giulia Galli

ALCC-2014

Impact and Approach

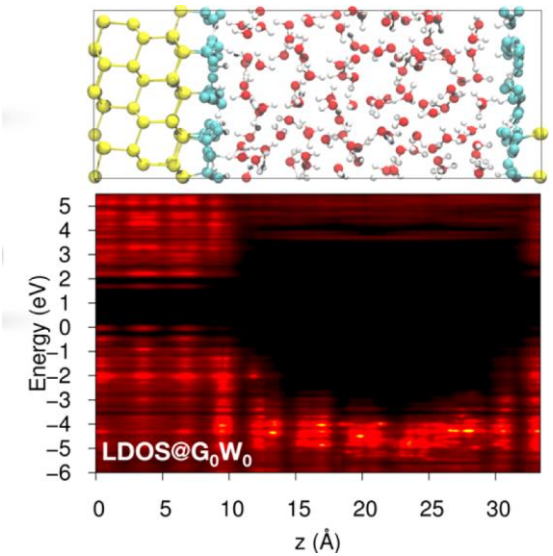
- Solid/liquid interfaces play a key role in solar conversion processes, e.g. in photocatalysis of water
- Techniques used: ab initio molecular dynamics (AIMD), first principle electronic structure simulations using density functional theory (DFT) and many body perturbation theory (MBPT).
- The use of the BG/Q architecture at ALCF has greatly impacted this project, since all simulations performed in the project were at a scale not doable on other platforms.

Accomplishments

- This project supported the development of the large-scale MBPT software West, and several improvements and scalability tests of the AIMD code Qbox.
- We computed the electronic structure of solid/ liquid interfaces using DFT+MPBT; we carried out calculations for systems of unprecedented size, with ~2000 electrons; these calculations were made possible by algorithmic and software optimization developments.
- The WEST & Qbox software can be used to investigate a variety of properties of complex and heterogeneous materials.

ALCF Contributions

- The Catalyst Chris Knight has offered technical support by facilitating and optimization the submission of productions runs.



DFT+MBPT electronic structure of a model functionalized Si / liquid water interface.

Cosmic Frontier Computational End-Station

Salman Habib

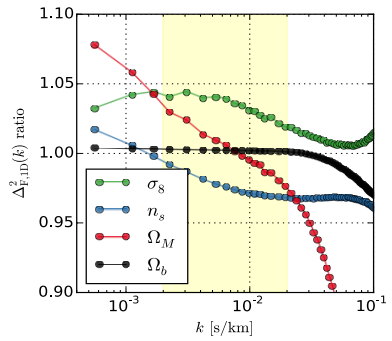
ALCC-2014

Impact and Approach

- Lyman-alpha forest simulations on Edison using the Nyx code, largest such suite ever carried out
- Finalized and analyzed the Outer Rim simulation on Mira, one of the largest cosmology simulations ever carried out – the very large number of particles required a large HPC resource such as Mira to carry out the computations
- Reionization investigations with the AMR code ART, again one of the biggest simulation runs in this area of research

Accomplishments

- Exploration of the cosmology dependence of 1d flux power spectrum, in preparation for the upcoming DESI survey
- Predictions for forthcoming 21cm experiments
- Investigation of epoch of cosmic reionization
- New set of strong lensing images
- One of the largest cosmology simulations ever carried out



ALCF Contributions

- Hal Finkel, Adrian Pope and Tom Uram have been essential for optimizing the analysis tool suite for HACC

Figure: 1-d flux power spectra for different cosmologies from the Nyx simulation set.

Validation Studies of Gyrokinetic Simulations to Understand the Coupling of Ion and Electron Scale Turbulence in Tokamak Plasmas

C. Holland, Lead PI

ALCC-2014

Impact and Approach

- Simulations help us understand the physics that sets performance of fusion experiments such as ITER
- We use an nonlinear initial value code to calculate dynamics of turbulent fluctuations in ion and electron distribution functions and the resulting particle, energy, and momentum fluxes
- Problem is 5D+time (3 config. space, 2 vel. space), nonlinear, requires simultaneous resolving spatial and temporal dynamics each spanning 3 or more orders of magnitude (e.g. 75M gridpoints)

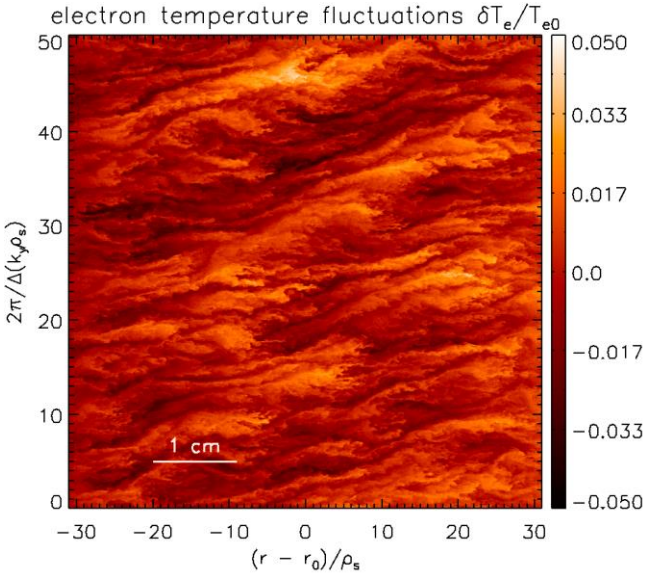
Accomplishments

- Simulations demonstrated that short wavelength turbulence can drive experimentally-relevant levels of transport, but is suppressed by strong long-wavelength turbulence

Visualization of multiscale electron temperature fluctuations using input parameters based upon a DIII-D tokamak discharge

ALCF Contributions

- Tim Williams helped optimize new CGYRO code for capacity-scale computing which will enable more efficient exploration of this issue in future studies.



Composite Higgs Theory Beyond the Standard Model

Julius Kuti

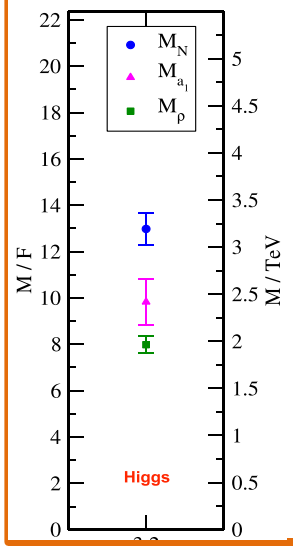
ALCC-2014

Impact and Approach

- The international LatHC collaboration with lead PI Julius Kuti tested a viable candidate theory for the explanation of the recently discovered Higgs particle. This effort potentially could replace the elementary Standard Model Higgs and reveal the nature of new constituents responsible for its origin.
- The team developed highly optimized code and performed very large-scale lattice gauge simulations using the best code world-wide for BG/Q deployment on Mira.
- Multi-rack running on the BG/Q was important for the science goals of the project.

Accomplishments

- The team developed the new composite Higgs theory for new predictions of the upgraded Large Hadron Collider at Cern, Geneva, Switzerland. They identified a low-mass scalar particle that could act as the Higgs impostor, if the theory remains successful.
- Predicted spectrum for LHC:



ALCF Contributions

- ALCF staff contributed to the science with regular technical support and advice to accomplish our science goals.
- Special thanks to our catalyst James Osborn had been outstanding throughout the year-long campaign. James had been always there for us to provide help, advice, know-how.
- Particular thanks to Ray Loy who on the system side helped so much with our early problems booting properly working partitions in our multi-rack Mira runs.

Simulation of Large Hadron Collider Events Using Leadership Computing

PI: T. LeCompte

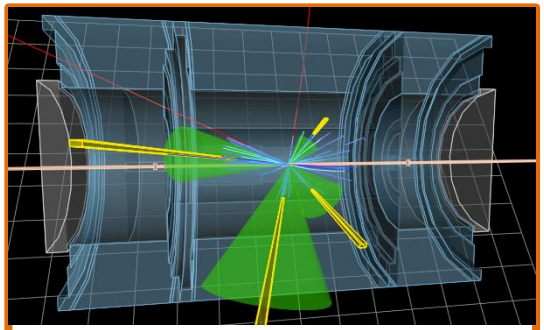
ALCC-2014

Impact and Approach

- The ATLAS experiment at the Large Hadron Collider relies on comparison between simulated and reconstructed events. Generating these events on Mira has advanced the time to science by 12-18 months.
- We take single-threaded tasks, run them as separate MPI ranks, with an initial step of coordinating input parameters, and a final step of aggregating the output.
- ATLAS' overall needs are roughly 1 billion x86-hours per year. This award covered 6% of a year's worth of computing. If we were a country, we would be the 7th largest. This only "fits" in capability partitions.

Accomplishments

- Details of the scientific impact will need to wait until the data is collected (0.1% is on tape so far) but 49% of ATLAS papers from the previous detector period used the equivalent data set.
- We were able to generate events that were too complex for our standard production.



One of the two billion simulated events
produced by Mira for ATLAS

ALCF Contributions

- We would not have been able to run at scale without the assistance of Tom Uram. This was a constant battle, with new fronts opening whenever we went to a larger partition. Today we can run at 48K in –c64 mode; we choose 16K partitions for better throughput. Tom received an ANL Pacesetter award for this work.
- Venkat Vishwanath and our catalyst Hal Finkel were instrumental in understanding and overcoming performance issues.
- The overburn policy made it possible to do 7x the science originally proposed.

Predictive Large-Eddy Simulation

Parviz Moin

ALCC-2014

Impact and Approach

•Predictive computing tools enable cost- and fuel-efficient design of aircraft and jet engines

•Demonstrating Large-Eddy Simulation tools on real geometries at flight Reynolds numbers with CharLES is crucial step towards use of HPC in aircraft industry

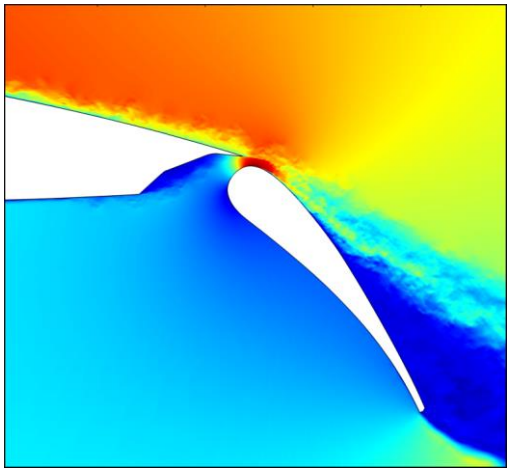
•Aircraft wings/engines are large and complex integrated, engineering systems. Turbulent flow over wing surfaces and outside fuel injectors has just recently become computable on leadership resources at ALCF using unsteady LES with wall models and fuel/spray atomization models.

Accomplishments

•Validation of LES wall-models for actuators/airfoils with CharLES

•Coupling these internal/external aerodynamic flows hinges on this

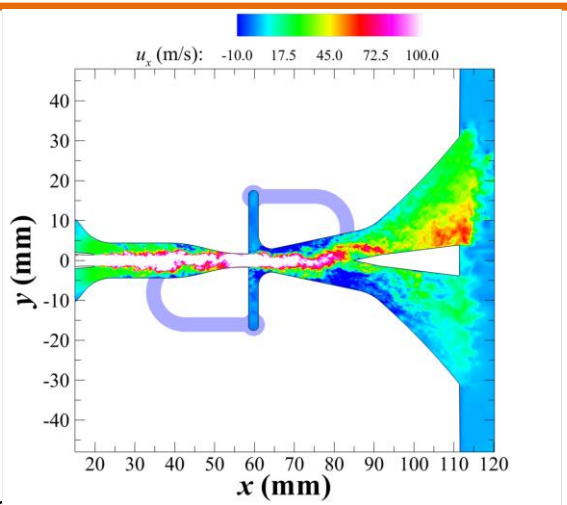
•V&V of 2-phase flow algorithms on unstructured grids in CharLES



Streamwise velocity contours near multi-element airfoil flap.

ALCF Contributions

•Ramesh Balakrishnan and Marta-Garcia Martinez helped our team communicate our work to the broader scientific community.



Streamwise velocity contours of Internal SaOB actuator flow (47M CVs)

Understanding secondary motions and their impact in modeling turbulent flows

PI: Hassan M. Nagib (Illinois Institute of Technology)

ALCC-2014

Impact and Approach

- Traditional computational flow studies assumed that if a duct is wide enough, it can be treated as infinitely wide (2D)
- This 2D assumption actually under-predicts friction/drag of the real flow
- Assessed friction dependence on duct aspect ratio and turbulence with Nek5000
- Discovered 3-dimensional effects present in turbulent duct flows which cause increase in friction for low aspect ratios due to interplay with duct geometry.
- Extended study to larger aspect ratios (14.4) and Reynolds numbers (Re_τ=360).

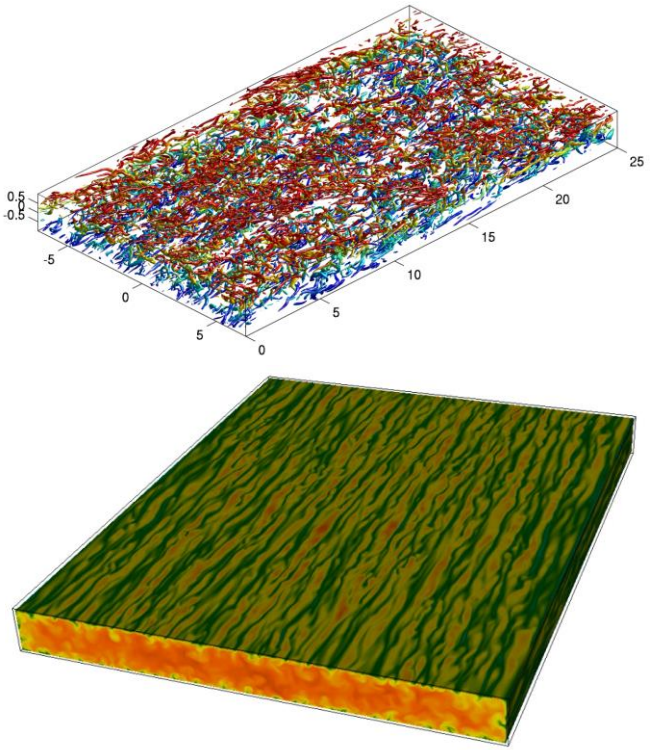
Accomplishments

- Gained deeper fundamental understanding of wall-bounded turbulence and what impacts it
- Shift CFD community towards looking at practical flows (3D)
- Results impact any practical flow calculation, i.e. drainage systems, ventilation systems, and combustion engines
- Deeper understanding will ultimately lead to improved prediction of flow physics and improved future designs (energy savings)

(Top) Coherent vortices in the AR=7 case and (bottom) instantaneous realization of the streamwise velocity field in the AR=10 case (both at Re_τ=180), Flow is from bottom to top, and the four walls have been removed to allow better visualization.

ALCF Contributions

- Nek5000 is a well-established code which has been tuned for BG/P and BG/Q machines in collaboration with ALCF staff over the past few years.



Nanostructure-enhanced Chemical Reactivity and Detonation in Energetic Materials

Aidan P. Thompson

ALCC-2014

Impact and Approach

- Scientific impact: The project supports the investigation of energetic materials. This work is providing fundamental insight into initiation mechanisms in energetic materials.
- Computational approach: Molecular dynamics simulations using ReaxFF (Reactive force field) reactive interatomic potential as implemented in LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)
- ReaxFF MD simulations on the required scale of 10 million particles can only be done on capability-class machines like Mira

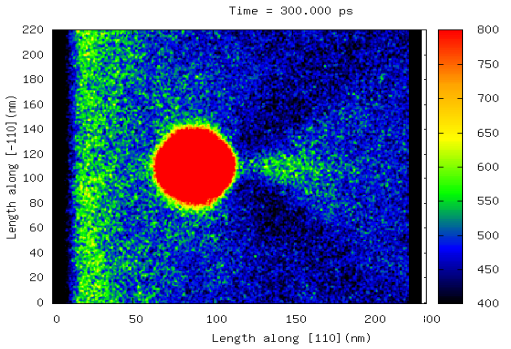
Accomplishments

- Spherical and cylindrical voids have similar effects on hot spot formation and initiation in energetic materials under shock conditions, although averaged hot spot temperature is somewhat lower for cylindrical voids.
- We observed the formation of a secondary hot zone located beyond the primary hot spot. Its formation may be attributable to the secondary shock wave generated when upstream void fragments collide with the downstream void surface.

ALCF Contributions

- Nichols Romero assisted in porting the Kokkos version of ReaxFF in LAMMPS to Mira

Caption: A triangular secondary hot zone forms beyond the circular-shaped primary hot spot



Delivering the Department of Energy's next-generation high-resolu Earth system model

PI: Peter Thornton

ALCC-2014

Impact and Approach

- Added the ability to make human system predictions to a coupled climate-biogeochemistry Earth System Model (ESM)
- Ran simulations with the ESM in a mode that allows explicit comparison with atmospheric observations
- Fully-coupled model of atmosphere, ocean, sea ice, and land, including ocean and land ecosystems. Horizontal resolution of simulation grid as fine as ¼ degree.
- New human dimension component includes prediction of fossil fuel emissions, land use, and agricultural comodity prices under a range of future policy scenarios.

Accomplishments

- Incorporation of explicit human dimensions component in an ESM drives significant changes in predicted fossil fuel emissions and agricultural commodity prices, compared to the standard approach in which climate model and human dimensions model are run asynchronously and with one-way coupling only.

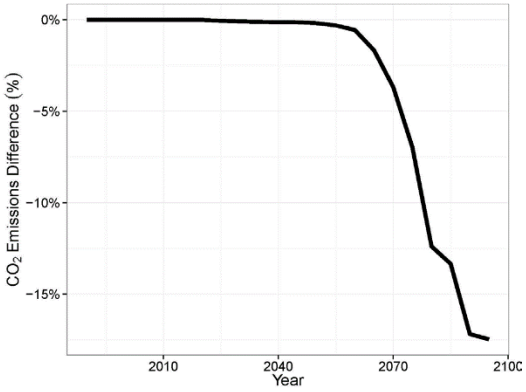


Figure caption: Difference in fossil fuel CO_2 emissions as a result of biospheric change feedback, shown as a percentage change between the two-way synchronous coupling and one-way asynchronous coupling simulations.

ALCF Contributions

- The ALCF point of contact for Science Support (Katherine Riley) has been very helpful in getting us started, holding telecon presentations for project staff to introduce them to the various resources and management tools.
- We have had great responsiveness from the accounts service team as we added numerous project members, and as we managed renewals of accounts and requests for additional space.

Influence of Morphology on Proton Transport Exchange Membranes: Gregory A. Voth (U. Chicago)

ALCC-2014

Impact and Approach

- Understand controlling factors for charge transport to guide development of improved energy storage materials.
- A reactive molecular dynamics method is used to simulate proton transport within water channels of polymer membranes with different internal structures (morphology).
- Goal is to build membrane morphologies that best match experiments.
- This study requires long simulation times with many system conditions to model (e.g. hydration level, polymer, morphology, concentration).

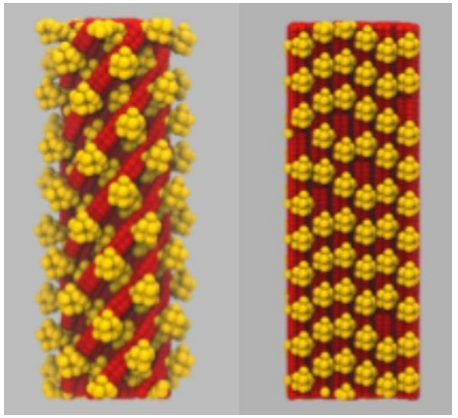
Accomplishments

- Comparison of transport properties from different membrane morphologies with experiment.
- Confirmed lamellae systems show faster proton transport than bundled morphology.
- Clear trend of increasing proton diffusion with hydration level.
- ALCC overburn policy enabled new sets of sodium mixture simulations.
- Rate of proton transport anti-correlated with surface area of water-membrane interface.
- Manuscript in preparation.

Right: Initial structures for backbone (red) and sidechain (yellow) particles in bundle (left) and lamellar (right) mophologies

ALCF Contributions

- Chris Knight (ALCF) is a co-developer of RAPTOR code and contributed to performance optimizations and bug fixes.
- Improvements to load-balance, removal of redundant FFTs, and improved rate of SCF convergence resulted in 1.7x speedup.
- Single-node optimizations in energy/force kernels resulted in further 45% speedup.



Understanding Helium Plasma Mediated Tungsten Response to better predict Performance in ITER

Brian D. Wirth, University of Tennessee

ALCC-2014

Impact and Approach

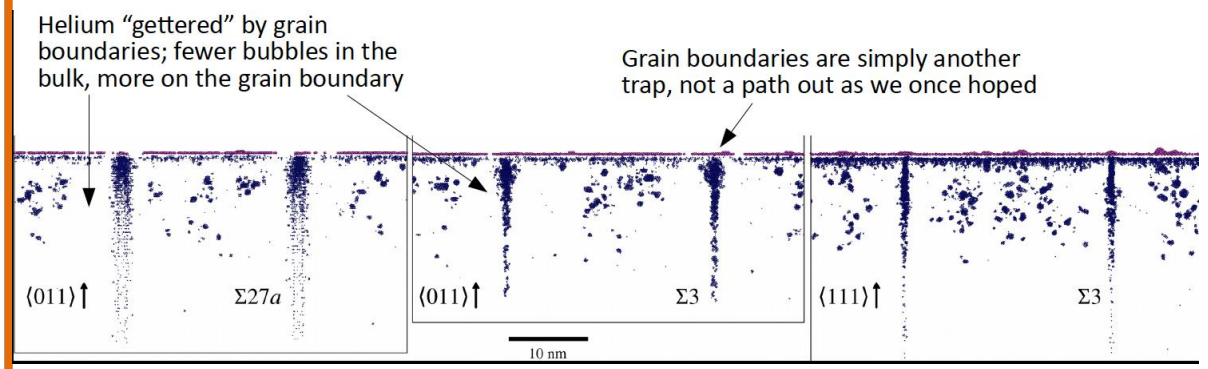
- Development of fusion energy requires improved knowledge of plasma surface interactions informing design of advanced components to bound the fusion plasma and extract heat
- Atomistic molecular dynamics simulations provide a computational microscope to visualize helium bubble formation and evolution kinetics that impact tritium retention and fusion reactor performance
- Small-scale computing introduces too fast dynamics into the system (e.g., gas implantation rates far exceed experimental reality)

Accomplishments

- Demonstrated, contrary to conventional wisdom, helum impurity atoms within tungsten are 'trapped' at grain boundaries with significantly slower rates of diffusion than in the grain interiors

ALCF Contributions

- Wei Jiang provided assistance with optimizing MD simulations and accessing additional time allocations



MD simulations showing helium (blue spheres) located below tungsten surfaces with grain boundaries that intersect the surface, as a function of surface orientation. Tungsten atoms displaced to the surface by the clustering phenomena are shown as purple spheres.