U.S. DEPARTMENT OF ENERGY | Office of Science

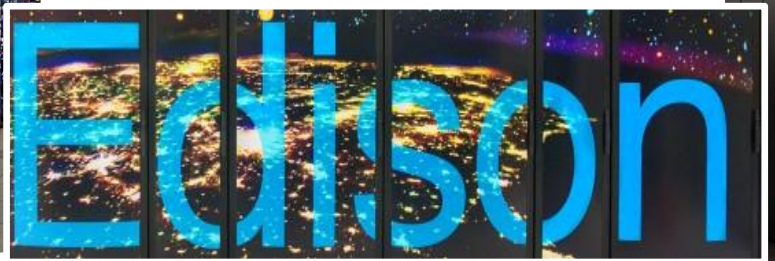
ASCR Leadership Computing Challenge

2013 ALCC Project Highlights

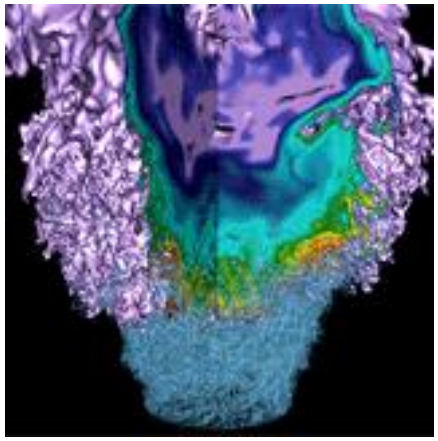
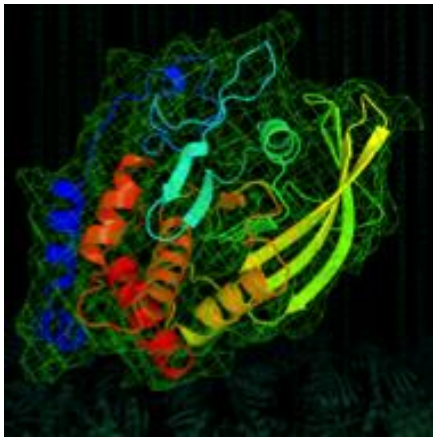
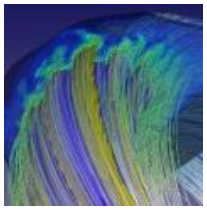
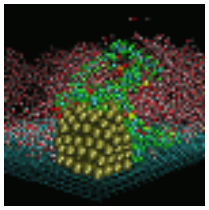
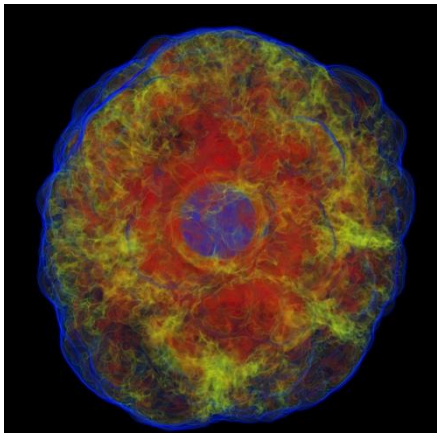
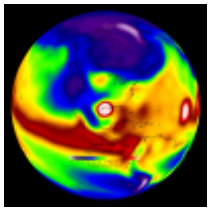
OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

BERKELEY LAB Lawrence Berkeley National Laboratory



NERSC ALCC Projects 2013


NERSC 40 YEARS at the FOREFRONT 1974-2014

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Chombo-Crunch: Advanced Simulations of Subsurface Flow and Reactive Transport Processes Associated with Carbon Sequestration

New Model Will Help Predict Stability of CO_2 Reservoirs

Scientific Achievement

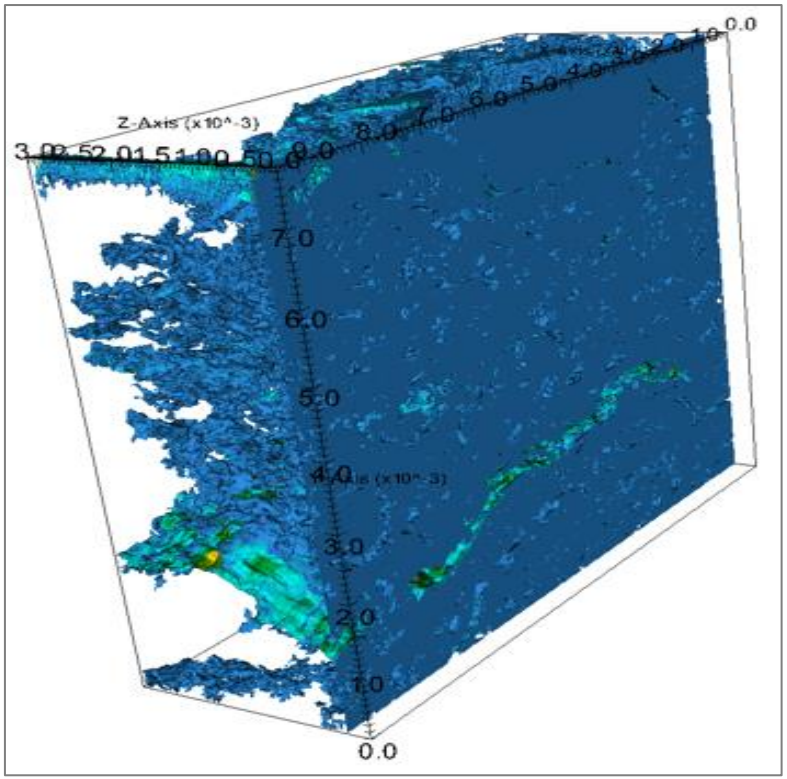
First-ever computer simulation of fully-resolved flow in fractured shale from image data.

Significance and Impact

The ability to simulate flow in shales with high resolution (less than 50 nm) 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 the incompressible Navier-Stokes equations 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.



Simulation of flow in fractured Marcellus shale using 60,000 cores of Hopper. Fluid velocity shown with 48-nm resolution. Sample courtesy of Tim Kneafsey (LBNL), imaged at Tescan USA.

Trebotich & Graves, *Comm. Appl. Math. Comp. Sci.* to appear (2015).

Work was performed at LBNL/CRD using NERSC

PI: David Trebotich (*LBNL*)

20M Hours

Computational Design of High-Efficiency Solar Thermal Fuel Materials

Scientific Achievement

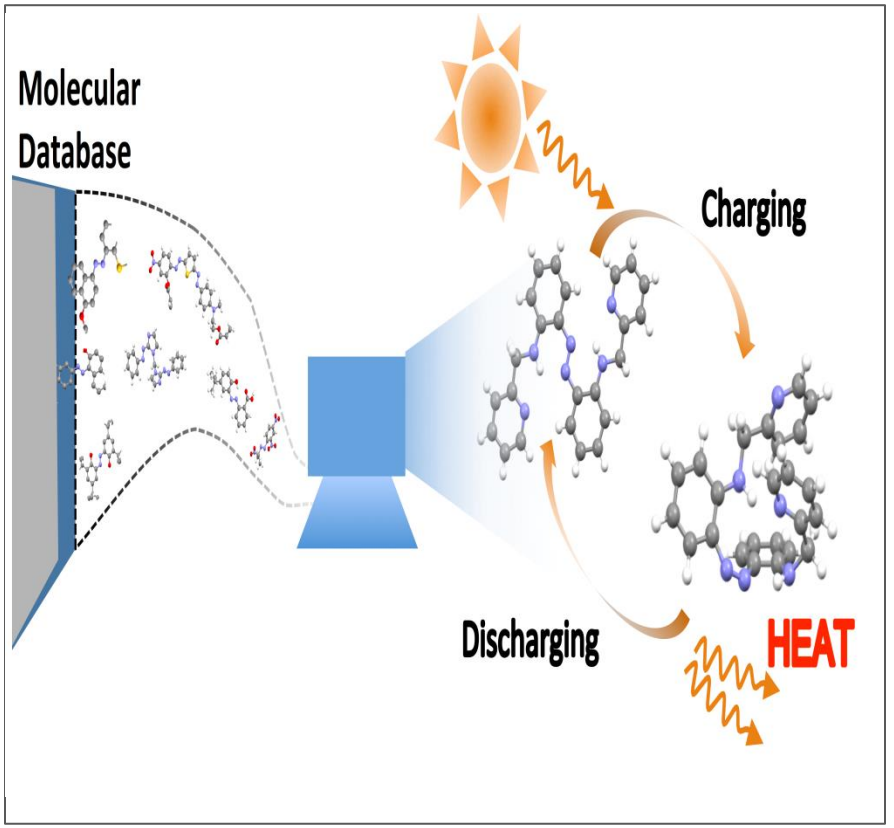
High-throughput simulations have revealed novel high-energy-density solar thermal fuel (STF) candidate materials as well as new materials design principles.

Significance and Impact

STFs may offer an emission-free and renewable solution for solar energy conversion and storage.

Research Details

- Focused on possible metastable structures of materials composed of earth-abundant elements
- Searched for potential isomerization patterns for a given molecule and then used *ab initio* simulations to calculate thermodynamics and optical properties
- Results also create deeper understanding of photoisomerization thermodynamics and may apply to other photochromism-related research fields, such as molecular switches and photo-responsive polymers.



Schematic showing the workflow involved in identifying new materials that store the energy of sunlight by changing the organization of atoms in a molecule, later to reorganize back to the original structure and release the energy as heat.

Liu and Grossman, *Nano Lett.* 14 (12), 7046-7050 (2014).

Work was performed at MIT using NERSC and NSF resources

PI: Jeffrey Grossman (*MIT*)

30M Hours

Study of the Internal Dynamics of ITER

Scientific Achievement

We have identified a mechanism where tokamak fusion plasmas exhibit an exceptionally stable, self-organized stationary state.

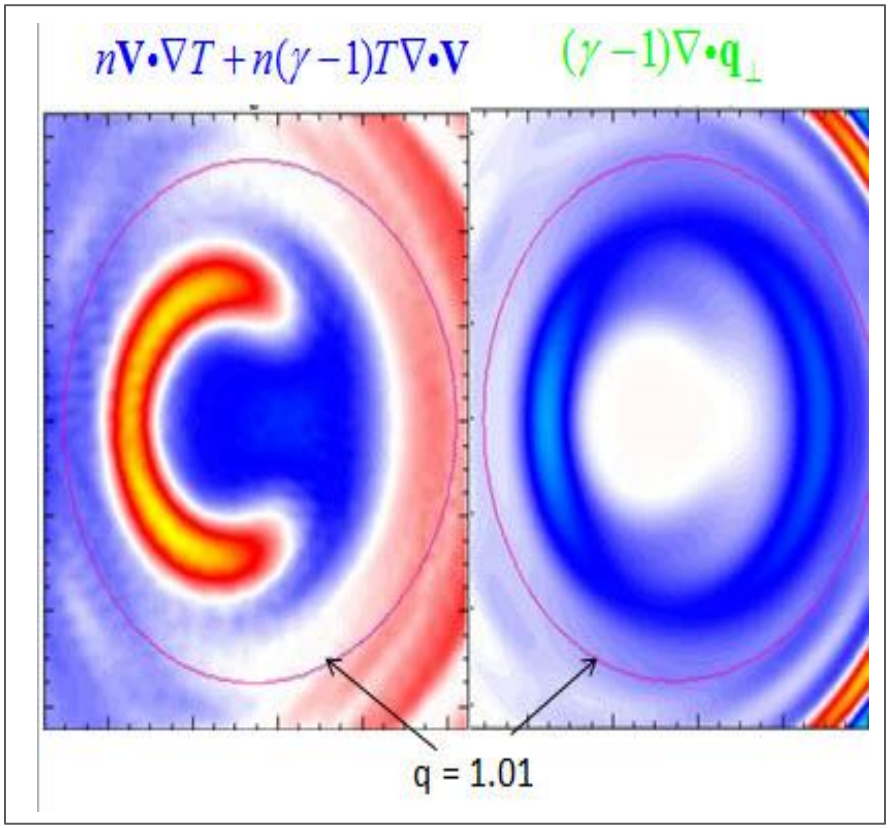
Significance and Impact

Tokamaks undergo periodic "sawtooth oscillation" reconnection events that can cause plasma disruption and abnormal termination. We have identified a parameter regime where these oscillations are absent, resulting in an exceptionally stable and quiescent discharge.

Research Details

- Dozens of long time simulations performed to explore parameter space using M3D-C1 toroidal 3D MHD code.
- New diagnostic output added to clarify the physics

Jardin, et al., Bull. Am . Phys. Soc. http://meetings.aps.org/link/BAPS.2014.DPP.BP8.24 (2014) (in preparation for Phys. Rev. Lett)



Terms in the energy balance for the temperature equation at one toroidal location in the plasma core for stationary state. Left frame shows terms driven by velocity. Right shows normal loss terms.

Work was performed at Princeton using NERSC

Investigation of Plasma Rotation Inversion and Profile Structure in Magnetic Fusion Experiments

Scientific Achievement

This work has led to a new physics discovery regarding the direction of intrinsic torque that drives toroidal rotation due to plasma turbulence.

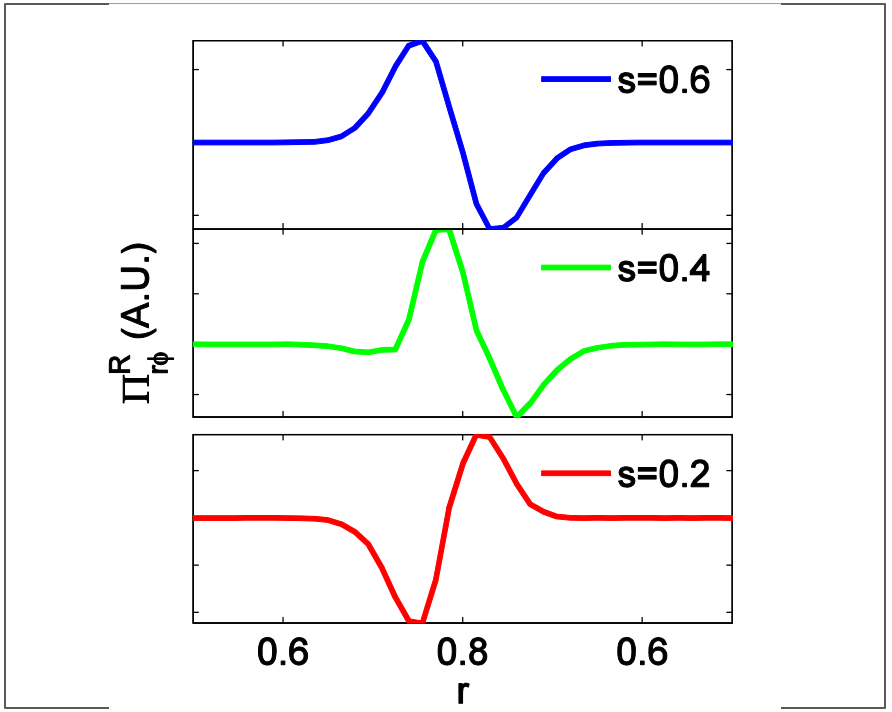
Significance and Impact

Understanding plasma rotation generation is critical for magnetic fusion experiments.

Simulation provides an explanation for the recent rotation reversal experiments on Alcator C-Mod

Research Details

- The Gyro-kinetic Tokamak Simulation (GTS) code was used on Edison to simulate the nonlinear evolution of global turbulence and the consequent toroidal momentum flux
- Systematic simulation study has discovered a critical magnetic shear for different type of turbulence, at which turbulence-generated torque for driving rotation changes direction
- GTS simulations of C-MOD experiments reproduced both intrinsic torque direction and critical magnetic shear value for torque reversal observed in the experiments
- Theoretical analysis has elucidated the underlying physics



As magnetic shear (s) decreases from 0.6 to 0.2, a specific momentum flux () that drives intrinsic rotation changes orientation, indicating the intrinsic torque reversal.

Publications and Invited talk (by Z. X. Lu, W. X. Wang, P. H. Diamond et al)
Effects of q-profile structure on intrinsic torque reversals, Invited talk at APS DPP, 2014, NI2.04
Intrinsic torque reversals induced by magnetic shear effects on the turbulence spectrum in tokamak plasmas, to appear in Physics of Plasmas
Effects of q-profile structure on intrinsic torque reversals, submitted to Nuclear Fusion

Work was performed at Princeton using NERSC

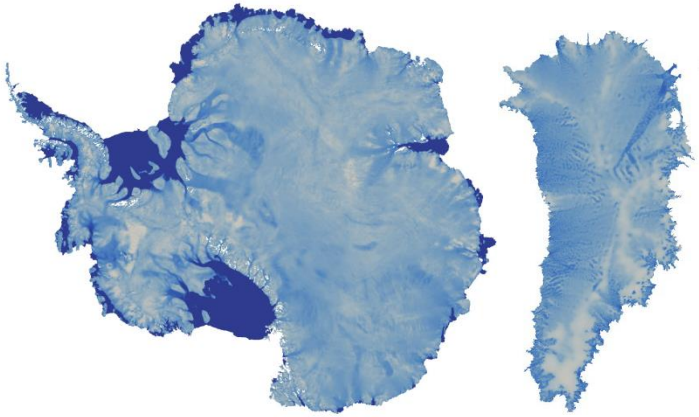
PI: Weixing Wang (*PPPL*)

5M Hours

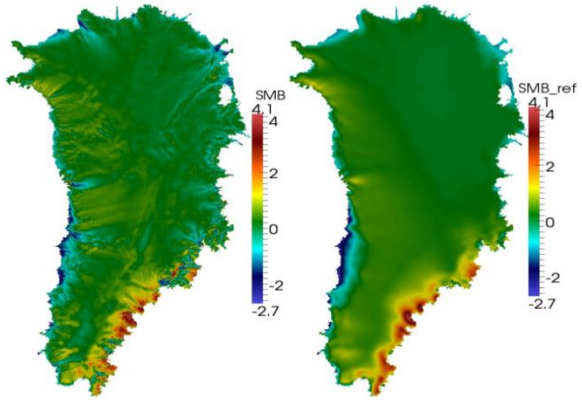
Projections of Ice Sheet Evolution : 1 of 3

Coupling of Ice Sheet and Climate Models

Below: Optimized basal friction maps for Antarctic and Greenland ice sheets (white = sticky, blue = slippery)



Below: Target climate model forcing (right) and model flux divergence (left). For smooth coupling to a climate model the two fields must be as similar as possible



M. Perego, S. Price, G. Stadler, *JGR*, **119**(9), 2014

Scientific Achievement

Developed and demonstrated a new, adjoint-based initialization procedure for ice sheet models

Significance and Impact

Inversion results will be used for sea-level rise projections from ice sheet models coupled to Earth System Models

Research Details

- Optimal ice sheet model initialization needed to perform future predictions of sea-level rise
- Inversion is done for basal friction and bedrock topography fields to achieve both a smooth coupling with climate forcing and a good match to observed velocities and geometry
- Requires solution of large-scale optimization problem (700K parameters using 2K processors)

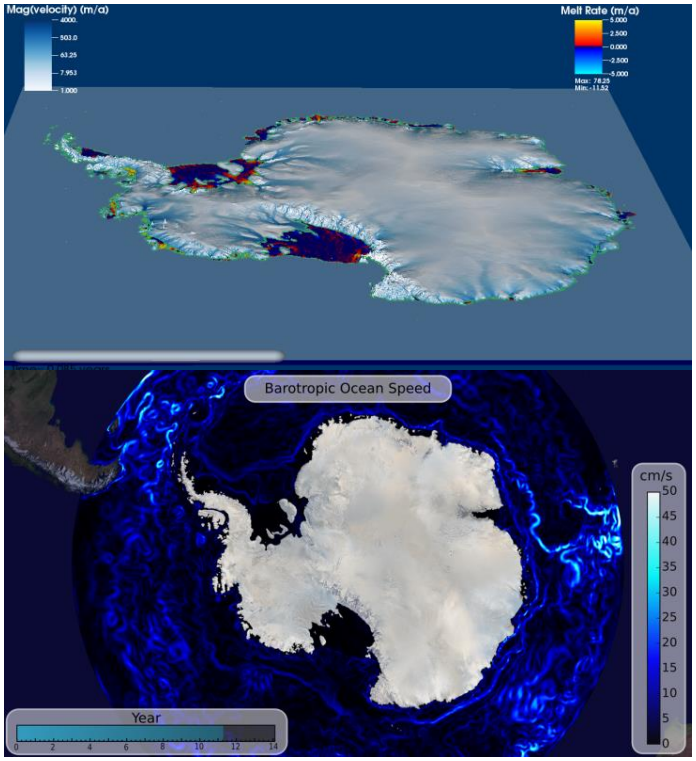
Work was performed at Sandia & Los Alamos National Labs and at the University of Texas

PI: Philip Jones (*PPPL*)

5M Hours

Projections of Ice Sheet Evolution 2 of 3:

POPSICLES: High-Resolution Coupled Ice Sheet & Ocean Modeling



Images from a POPSICLES simulation. *Top:* Antarctic ice sheet geometry colored with ice velocities (light blue) and ocean-model-produced melt rates beneath floating ice shelves. *Bottom*: Southern-ocean velocities computed by POP2X

Scientific Achievement

First-ever coupled, high-resolution, ice sheet & ocean modeling of full Southern Ocean and Antarctic ice sheet

Significance and Impact

Understanding and accurately modeling the coupling between ocean circulation and Antarctica's vast floating ice shelves is essential for projections of Antarctica's ongoing and future contributions to sea level rise

Research Details

- POP2x Ocean Model: high-resolution (0.1°) POP2 ocean model modified to enable circulation under ice shelves
- BISICLES Ice sheet model: scalable, adaptive mesh refinement down to 500m resolution where needed to resolve important ice sheet dynamics
- Currently validating using idealized climate forcing

Work performed on NERSC's Edison by LBNL, LANL, and the Potsdam Institute for Climate Impact Research (PIK)

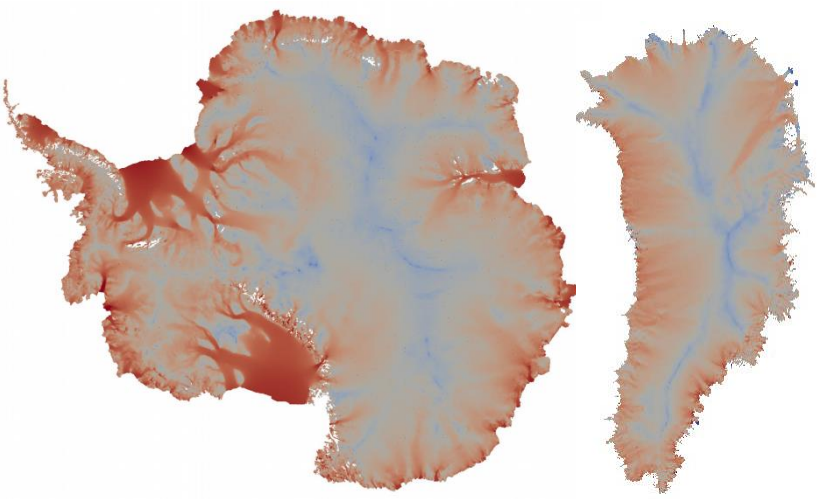
PI: Philip Jones (*PPPL*)

5M Hours

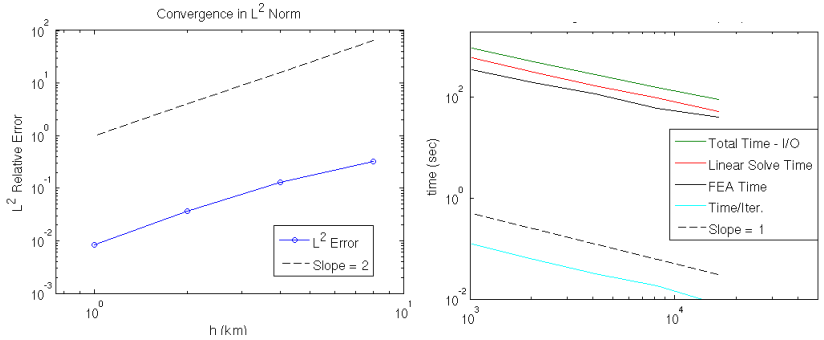
Projections of Ice Sheet Evolution : 3 of 3

Scalability and Convergence of the *Albany/Felix* Ice Sheet Model

Optimized surface velocities for Antarctica and Greenland



Convergence study (left) and strong scalability results for Greenland ice sheet simulations



Scientific Achievement

Demonstration of improved scalability and convergence of a next-generation ice sheet model

Significance and Impact

Albany/Felix will be used in future DOE Earth System Model simulations. Work performed assesses accuracy, efficiency, and robustness of the model in realistic ice sheet simulations

Research Details

- Demonstration of numerical scheme convergence with mesh refinement
- Implemented Multigrid preconditioner to improve efficiency and scaling
- Performed large-scale runs (up to 1.2B unknowns and 14K processors) demonstrating good scalability on realistic Antarctic and Greenland ice sheet problems

I. Kalashnikova, M. Perego, A. Salinger, R. Tuminaro, S. Price, M. Hoffman, *Geoscientific Model Development* (to appear)

Work was performed at Sandia and Los Alamos national labs

PI: Philip Jones (*PPPL*)
5M Hours

High Strength, Molecularly Thin Nanoparticle Membranes

Scientific Achievement

Simulations provided unprecedented molecular detail that cannot be obtained experimentally about why single-layer nanoparticles encoded with short organic chains are so surprisingly strong.

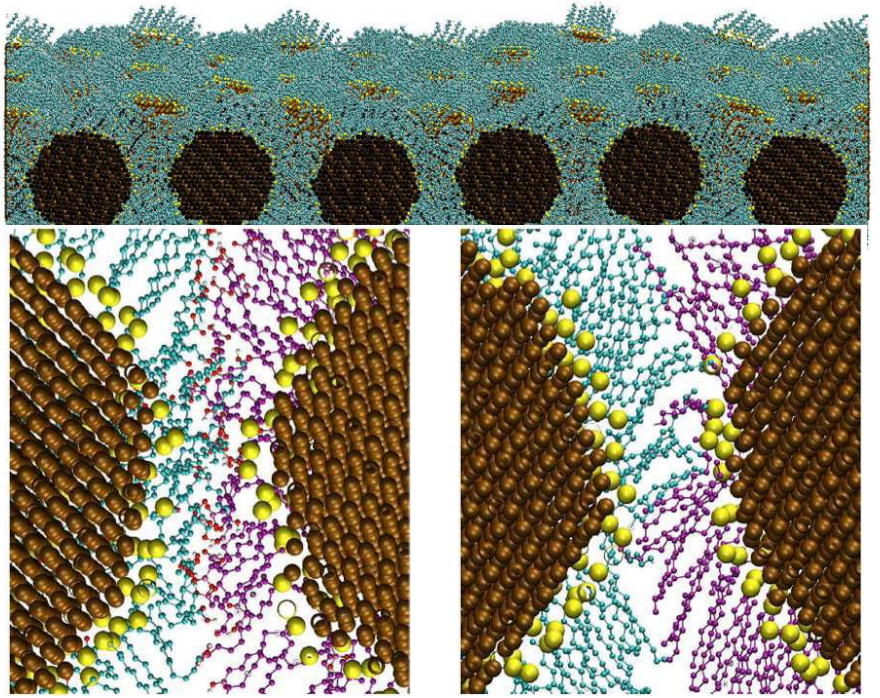
Significance and Impact

Because of their unusual strength, thin nanoparticles membranes have many potential applications, from sensor arrays to nanoscale filtration. Current study resolved the fundamental mechanisms underlying their unique mechanical strength.

Research Details

- Multi-million atom molecular dynamics simulations of alkanethiol-coated gold nanoparticle membranes were carried out to simultaneously measure nanoscale interactions while directly comparing membrane properties to experiment.
- By replicating experimental conditions, nanoparticle membranes at a water-vapor interface were made and then water removed to form free-standing membranes.
- Mechanical tests of the resulting membranes were then made and compared to experiment
- Resulting insights can be used to design nanoparticle membranes with more finely tailored properties.

K. Michael Salerno, Dan S. Bolintineanu, J. Matthew D. Lane, and Gary S. Grest, Physical Review Letters 113, 258301 (2014)



Top: angled side view of CH_3-terminated dry membrane prior to deformation. H atoms are represented in white, C: cyan, Au: brown, and S: yellow. Bottom: close-up of COOH terminated (left) and CH_3-terminated (right) nanoparticles. Hydrogen atoms have been omitted except in the COOH end group. C atoms on the left NP are colored cyan while those on the right are colored purple.

Research was carried out at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Work supported by Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) at NERSC.

PI: Gary S. Grest (*SNL*)

40M Hours

Simulating Cosmological Lyman-Alpha Forest

Scientific Achievement

We have produced two of the world's largest simulations of the Lyman alpha forest statistics in spectrum of quasars.

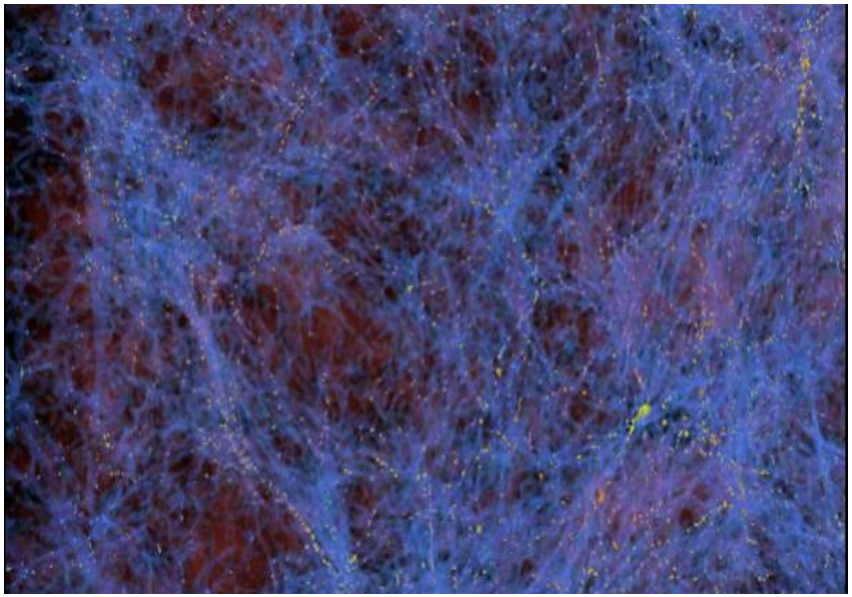
Significance and Impact

Accurately simulating intergalactic medium is crucial for constraining cosmological parameters with spectroscopic quasar surveys, like BOSS and DESI. Simulations performed under this ALCC serve as the "gold standard": they are the first to model cosmologically significant volumes and simultaneously resolve small density fluctuations relevant for the Lyman-alpha forest.

Research Details

- Used Nyx N-body + hydrodynamics code on NERSC's Edison
- Demonstrated 1% accuracy for all relevant statistics, like the flux power spectrum.
- Explored two different Ultra-Violet Background models commonly used in modern literature.
- Full simulation data will be available to the wider scientific community.

One paper published (Lukić et al. 2015, MNRAS, vol. 446, p. 3697), one submitted, more in preparation. Several invited presentations.



In blue we show regions of high Lyman-alpha absorption, while red are void places of low absorption. Yellow are regions corresponding to galaxies: locations where gas becomes dense and cold enabling the star formation.

Work was performed at LBNL/CRD using NERSC

PI: Zarija Lukic (*LBNL*)

24M Hours

Modeling Helps Elucidate Mechanism of DNA Repair

Scientific Achievement

We identified important structural and energetic details governing the base extrusion mechanisms in glycosylases - key enzymes involved in DNA repair that helps to maintain genomic integrity.

Significance and Impact

DNA repair is important because of interest in microbial genome and metabolic responses to environmental stresses such as ultraviolet radiation, ionizing radiation and oxidative stress.

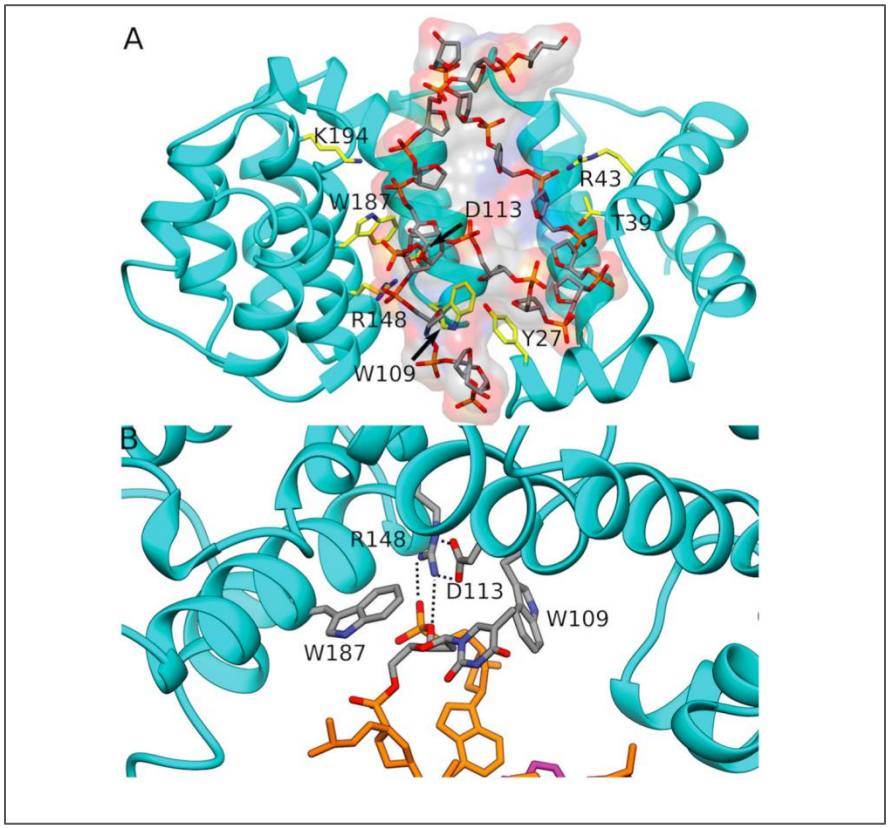
Research Details

- We delineated the role of DNA sculpting in the unusual base extrusion mechanism of the DNA repair enzyme alkylpurine glycosylase D (AlkD)
- We characterized base extrusion in thymine DNA glycosylase (TDG), which plays critical roles in base excision repair and epigenetic regulation
- We pushed the application of chain-of-replicas path optimization methods to understand these important biological mechanisms

• Kossmann, B. & Ivanov, I. PLOS Computational Biology (2014) 10, e1003704. doi: 10.1371/journal.pcbi.1003704

• Yan, L., Yan, C., Su, H., Qian, K., Wofford, S., Zhao, X., Ivanov, I. & Zheng Y.G. J. Med. Chem. (2014) 57, 2611–2622, doi: 10.1021/jm401884z

• Xu, X., Guardiani, C., Yan, C. & Ivanov, I.. Nucleic Acids Research (2013) 41, 10020-10031, doi:10.1093/nar/gkt810.



AlkD recognizes DNA through HEAT repeat motifs. A) Overall architecture of the AlkD-DNA complex with residues contacting the DNA backbone shown explicitly and labeled; B) The mode of recognition of the extrahelical thymine base opposite to the 3 mA lesion.

Work was performed at Georgia State using NERSC

PI: Ivanov Ivaylo (Georgia State University)

3M Hours

Coupled Hydro-Geophysical Modeling Improves Understanding of Hanford 300 Area Groundwater

Scientific Achievement

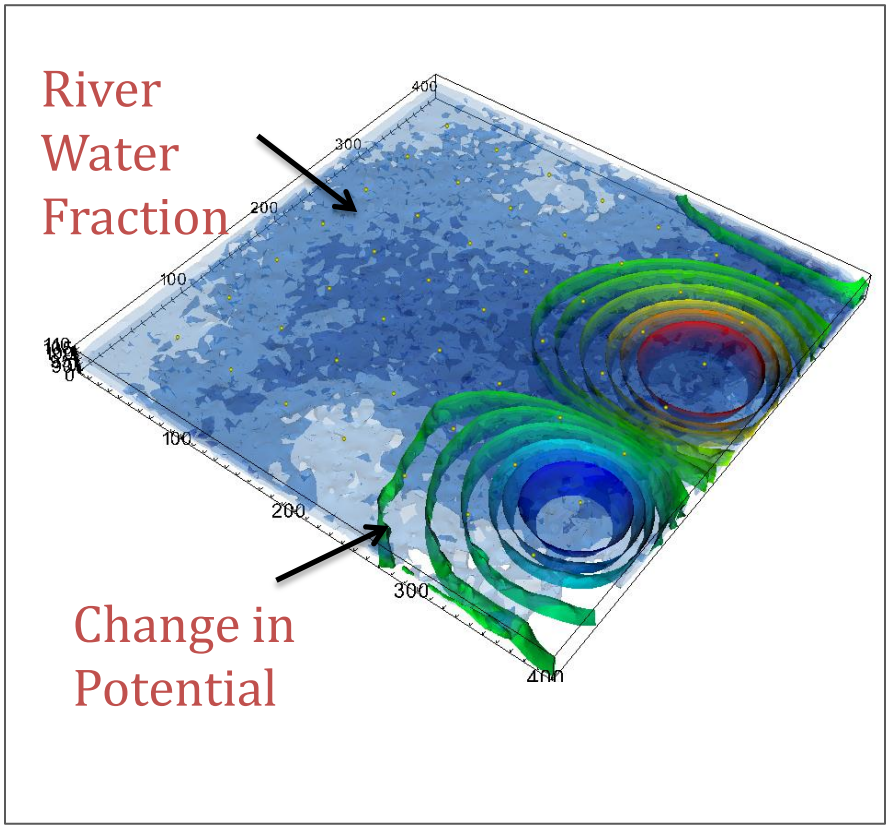
We have coupled the flow and transport HPC code PFLOTRAN with a geophysical code E4D to enable hydrogeophysical data assimilation.

Significance and Impact

We successfully assimilated images taken by time-lapse electric resistivity tomography to characterize heterogeneous aquifer permeability at the groundwater-river water interaction zone at the Hanford site, which provided essential information for modeling biogeochemical processes in the zone.

Research Details

- Coupled PFLOTRAN and E4D to provide key modeling capability of multi-physics processes, parallel efficiency, and multi-realization simulation capability for data assimilation.
- Implemented ensemble-based Bayesian data assimilation methods to use multiscale and multi-type data for characterizing heterogeneity and reducing uncertainty in model predictions.
- Efficient parallel HPC implementation



Simulated River Water Fraction Field by PFLOTRAN That Was Passed to E4D for Simulating The Change in Electrical Potential Field

Chen X, TC Johnson, GE Hammond, and JM Zachara. " Coupled Hydrogeophysical Inversion for Characterizing Heterogeneous Permeability Field at a Groundwater-River Water Interaction Zone" Pres. at American Geophysical Union Fall Meeting, San Francisco, CA on December 19, 2014.

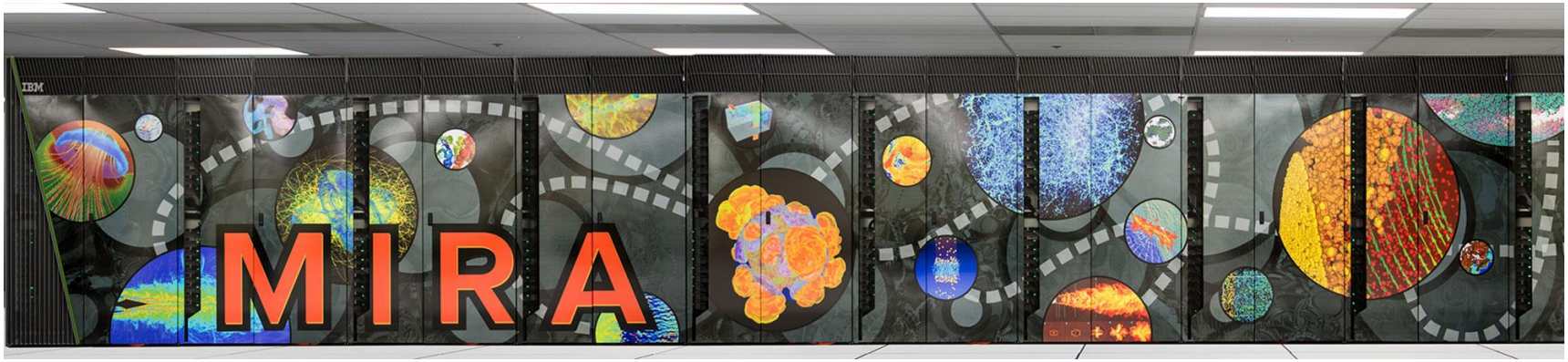
Work was performed at PNNL using NERSC

PI: Glen Hammond (*PNNL*)

16M Hours

ALCF Projects 2013 ALCC

Argonne Leadership
Computing Facility



Protein Binding and Interaction Analysis of Human Pathogen Protein Targets

PI: Andrew Binkowski, Argonne National Laboratory.

Argonne Leadership Computing Facility

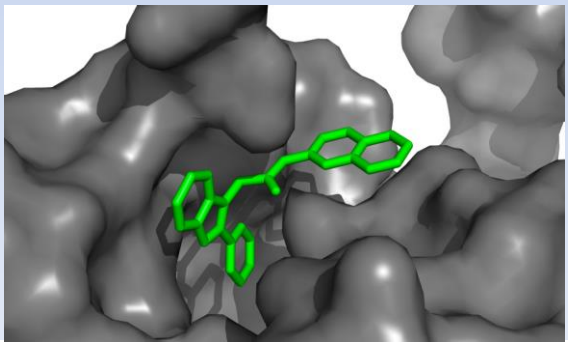
ALCC Award: 22,800,000 hours

Science and Approach

Computational discovery studies of high-value biomedical targets such as

- human pathogens
- bioterrorism agents
- human disease related proteins

(Left) The bound inhibitor pose reveals additional space in the cavity.



Key Impact

- Used novel Free Energy Perturbation Replica-Exchange Molecular Dynamics with respect to the thermodynamic parameter (FEP/-REMD) method
- Conducted unprecedented large-scale studies to evaluate and benchmark the higher order protein-ligand binding free energy calculations on Blue Gene P and Q
- PI identified a select pool of compounds as potential candidates

ALCF Contributions

Ported existing pipeline from Blue Gene P to Q. This included assistance in

- compiling software
- managing storage
- evaluating best practices
- exploring opportunities for optimizations

Different compiler options were explored which led to ~30% speed improvement.

Argonne NATIONAL LABORATORY

Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions

Argonne Leadership Computing Facility

ALCC Award: 250,000,000 hours

PI: Robert A. DiStasio Jr., Princeton University

Science and Approach

- Highly accurate benchmark atomistic simulations of liquid water and aqueous ionic solutions that are most relevant to the design of novel clean energy materials.
- Balanced treatment of electrons and nuclei—density functional theory based *ab initio* molecular dynamics (AIMD) in conjunction with the Feynman path integral (PI) technique.
- Computationally demanding calculations were made possible by use of algorithms customized for Mira.

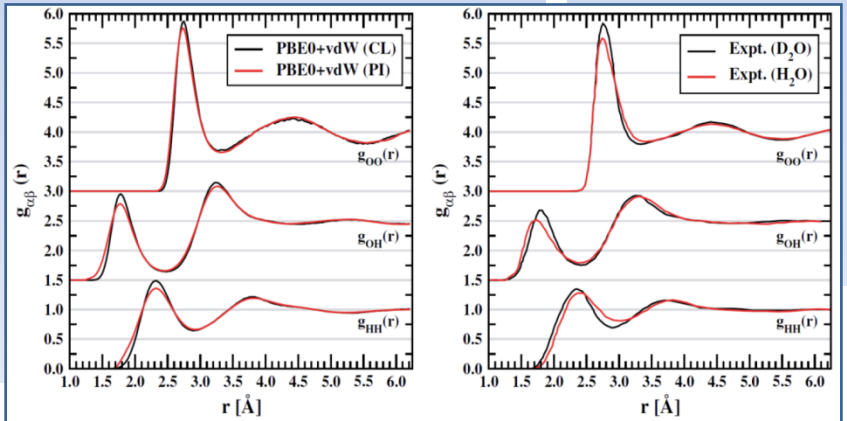
Key Impact

- Anomalous density ordering between ice and liquid is now accurately predicted.
- PI-AIMD simulations capturing subtle isotope effects in structure of liquid water.
- Proton transfer rates obtained from simulations of aqueous ionic solutions are in excellent agreement with experiment.

ALCF Contributions

- In collaboration with Alvaro Vazquez-Mayagoitia, a highly efficient Poisson solver was developed which reduces the computational cost of these simulations.

(Center and Right) Radial distribution functions of liquid water from theory (classical (CL) and path integral (PI) AIMD simulations) and experiment.



Argonne NATIONAL LABORATORY

Large Eddy Simulation of SFR Assembly Inlets

PI: Paul Fischer, Argonne National Laboratory
James Tallman, General Electric, Global Research.

Argonne Leadership Computing Facility
ALCC Award: 60,000,000 hours

Science and Approach

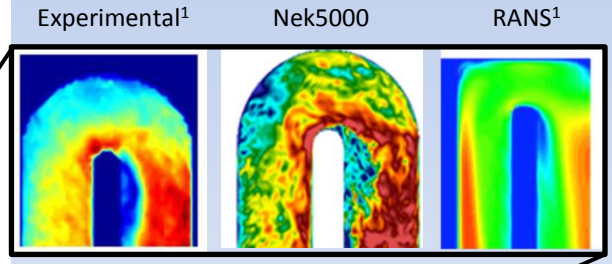
- Rescoped in October 2013 for particle transport in turbine internal cooling passages
- Direct Numerical Simulation and Large Eddy Simulation of Turbulent Flows
- Discrete Element Lagrangian Particle Tracking
- Spectral Element Method Solver

Key Impact

- Improved understanding of flow physics around turbulators
- Features of flow in tipturns, in particular recirculation and influence of flow on first upstream turbulators
- Better understanding of particle transport characteristics in these systems

ALCF Contributions

- In prior years, ALCF staff helped port and optimize Nek5000.



[1]Booten, 2006

Argonne NATIONAL LABORATORY

Predictive full-scale simulations of fast ignition of fusion targets

PI: Frederico Fiuza, Lawrence Livermore National Laboratory

Argonne Leadership Computing Facility

ALCC Award: 19,500,000 hours

Science and Approach

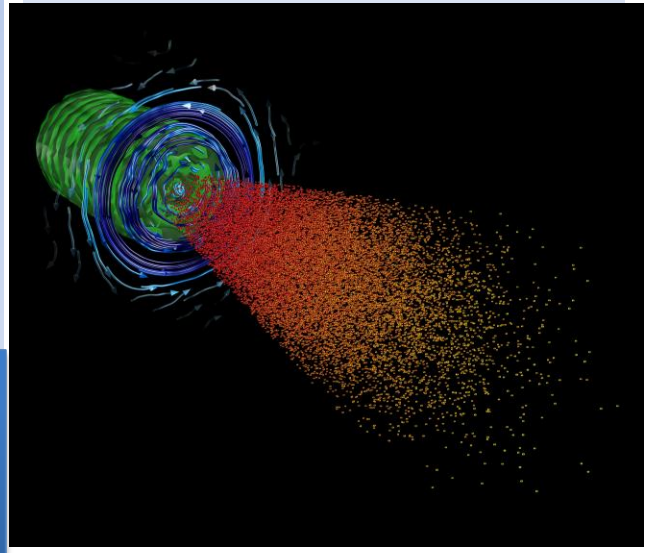
- Fast ignition: short, high-power laser pulse generates fast electrons that heat and ignite already-compressed fusion fuel pellet.
- Understanding energy transfer from laser to electrons in the fuel (plasma) is critical for success of this fusion approach.
- 3D first principles simulations using particle-in-cell (PIC) code OSIRIS.

Key Impact

- Largest 3D simulations to date of laser-plasma interactions in fast ignition. Studied different plasma densities, laser intensities & wavelengths
- Results show fast electron divergence away from target center smaller than previous studies suggested. (<30° vs. 40°)
- This means the prospects for fast ignition are better than expected.

ALCF Contributions

- Helped compile, benchmark, tune thread use



(Right) Incoming laser pulse shown green, blue magnetic field lines at fuel plasma surface, orange fast electrons ejected.

Argonne NATIONAL LABORATORY

First principles investigations of adsorbate-metal interactions using QMC

Argonne Leadership Computing Facility

ALCC Award: 50,000,000 hours

PI: Jeffrey Greeley, Purdue University.

Science and Approach

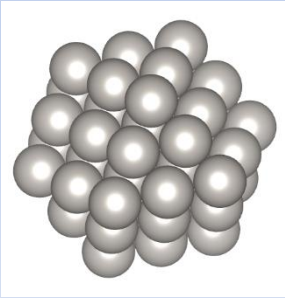
- Quantum Monte Carlo (QMC) calculations are applied to clusters and surfaces of platinum.
- Platinum is a transition metal that has numerous applications in catalysis and electrochemistry.
- QMC calculations provide unprecedented accuracy and benchmark results for platinum's structural and electronic properties.

Key Impact

- A new QMC pseudopotential for platinum was designed. This will enable future QMC calculation on more complex systems, e.g. catalysis on the platinum surface.
- QMC calculations have yielded accurate structural and energetic information on sub-nanometer platinum clusters, with applications to next-generation catalysis.

ALCF Contributions

- ALCF staff installed, maintained, and validated the QMCPACK code on ALCF resources.



(Right) A 55-atom Pt cluster that was studied using QMC calculations

Argonne NATIONAL LABORATORY

First-principle investigations of oxygen defects in metal/oxide/metal heterostructures

PI: Olle Heinonen, Argonne National Laboratory.

Argonne Leadership Computing Facility

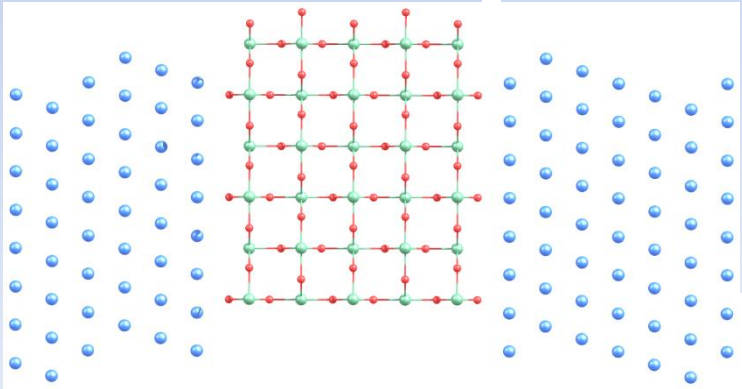
ALCC Award: 50,000,000 hours

Science and Approach

- Electronic structure and transport of oxide structure and microscopic mechanism of resistive switching in metal/oxide/metal heterostructures
- Quantum Monte Carlo (QMC) for high-precision calculations of complex oxides.
- Self-interaction corrected (SIC) density functional theory (DFT) calculations for studying electron transport .

Key Impact

- QMC calculations of Ti equation of state on Mira to validate QMC pseudopotentials for later use on Ti oxides
- Transport calculations of $Pt/TiO_2/Pt$ structures showed transition from conducting to insulating with increasing thickness of TiO_2



ALCF Contributions

- ALCF worked with developer to port TranSIESTA code to Blue Gene/Q.
- ALCF collaborated on Ti QMC calculations.

(Center and Right) Depiction of $Pt/TiO_2/Pt$ structure. Pt, Ti, and O are blue, red, and green spheres, respectively.

Argonne NATIONAL LABORATORY

Mock BOSS: Calibrating BOSS Dark Energy Science with HACC

PI: Katrin Heitmann, Argonne National Laboratory.

Argonne Leadership Computing Facility

ALCC Award: 45,000,000 hours

Science and Approach

- Large-scale surveys of the distribution of galaxies are carried out and will be used to unravel the mystery of dark energy.
- Very large cosmological simulations spanning different models will aid two major surveys, BOSS and DESI.
- We used the HACC N-body code to create cosmological laboratories in which different effects of major cosmological parameters on the distribution of galaxies can be studied.
- Only the largest HPC systems allow us to carry out such simulations in a timely fashion.

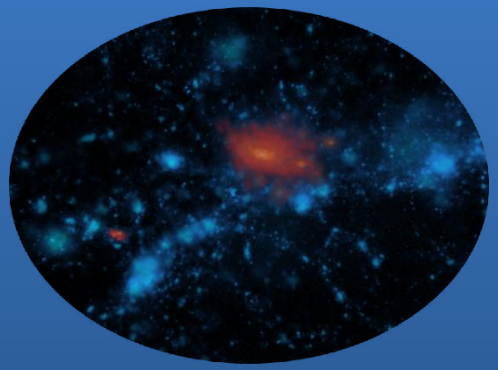
Key Impact

- Unique resource for studying the large-scale distribution of matter in the Universe encompassing more than 60 mock catalogs covering the full BOSS survey footprint.
- Enabling studies of the distribution of extreme objects in large surveys.
- Exploration of the dependence of the distribution of matter on cosmological parameters.
- Enabling studies of systematics effects on cosmological parameter estimation.

ALCF Contributions

- Staff assisted with visualization.

(Right) Dark matter distribution from one of our simulations. The red region highlights a very large cluster.



Argonne NATIONAL LABORATORY

Petascale Thermal Hydraulic Simulations in Support of CESAR

PI: Elia Merzari, Argonne National Laboratory

Argonne Leadership Computing Facility

ALCC Award: 20,000,000 hours (BG/P)
60,000,000 hours (BG/Q)

Science and Approach

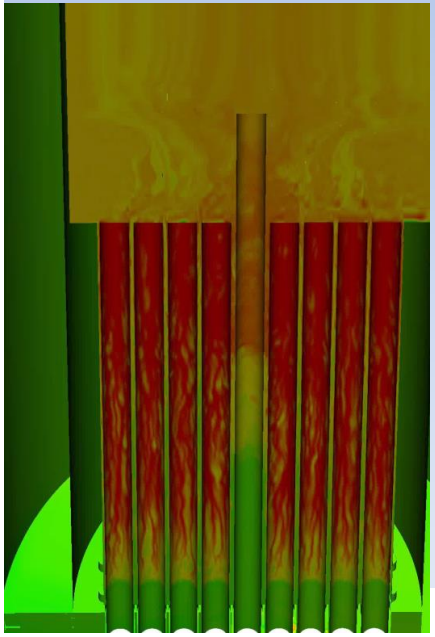
- Numerical simulations are an intrinsic part of nuclear engineering research and power plant design.
- CESAR (Center for Exascale Simulations of Advanced Reactors) team focuses on developing simulation tools and algorithms for exascale platform to solve large, difficult problems.
- Several reactor geometries were studied with Nek5000 to evaluate performance and identify issues.

Key Impact

- Detailed simulation of 37 pin nuclear fuel bundle shed light on physics of turbulence in that geometry.
- Simulation of MASLWR experiment resulted in conclusion that transients must be accelerated to make the problem computational tractable.
- Simulation of AREVA grid spacer design was compared to lower fidelity methods to compare cost and accuracy.

ALCF Contributions

- In prior years, ALCF staff helped port and optimize Nek5000.
- ALCF staff assisted with reservations on ALCF resources to meet critical project deadlines.



(Right) Temperature distribution in the MASLWR core computed using Nek5000 (frozen velocity)

Wall Modeling and Primary Atomization for Predictive Large-Eddy Simulation

PI: Parviz Moin, Stanford University.

Argonne Leadership Computing Facility
ALCC Award: 150,000,000 hours

Science and Approach

- Practical engineering and aeronautical applications need LES models to treat unresolved near-wall eddies & atomized fuel droplets on unstructured grids.
- New LES wall-models and two-phase flow algorithms in CharLES applied to multi-scale/physics applications: scramjets, fuel injectors and automotive mirror noise.
- LES modeling capabilities enable virtual testing and prototyping to reduce drag & improve fuel efficiency of complex geometry engines, aircraft & vehicles.

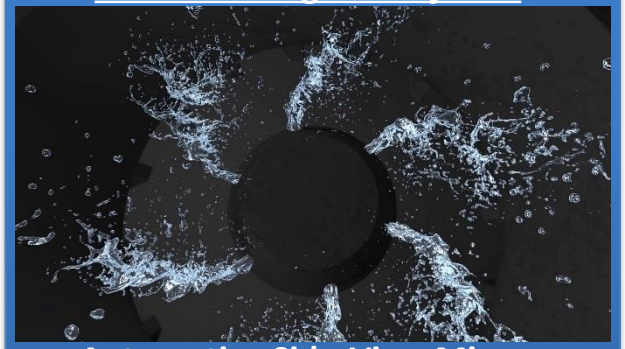
Key Impact

- New LES models reproduce flight & ground test experiments for HIFiRE scramjet engine; unprecedented numerical database and validation.
- Novel wall-model tested on side-view mirror, validated against Honda experiments.
- Unstructured, exactly mass conserving VoF/Lagrangian scheme applied to full fuel injector and validated with UTRC experimental data.

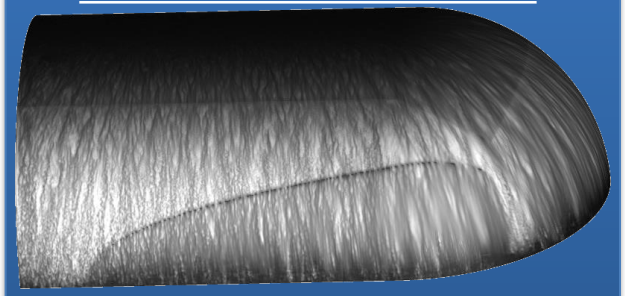
ALCF Contributions

- Improved parallel I/O and performance of CharLES

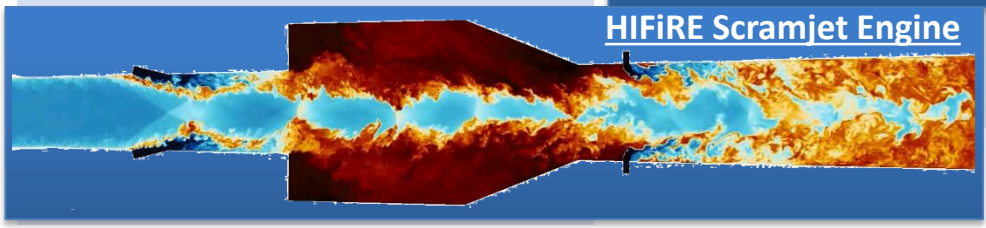
Entire Swirling Fuel Injector



Automotive Side-View Mirror



HIFiRE Scramjet Engine



Does a Turbulent Flow Ever Become Two-Dimensional?

PI: Hassan Nagib, Illinois Institute of Technology

Argonne Leadership Computing Facility

ALCC Award: 11,000,000 hours (BG/P)
2,000,000 hours (BG/Q)

Science and Approach

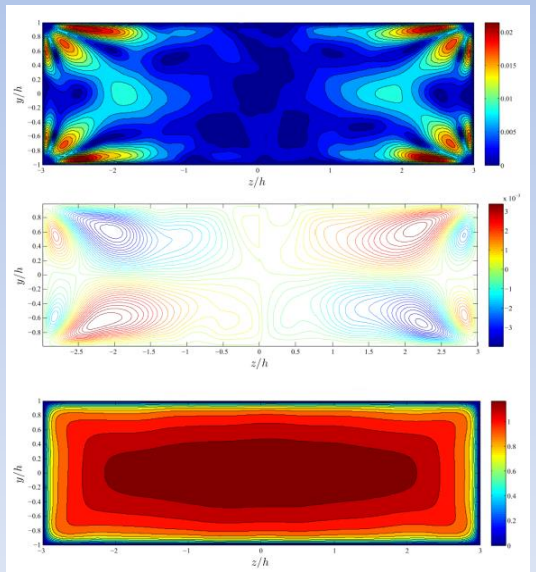
- Traditional computational flow studies assumed that if a duct is wide enough, it can be treated as infinitely wide (2D).
- This 2D assumption actually under-predicts friction/drag of the real flow.
- Assessed friction dependence on duct aspect ratio and turbulence with Nek5000.
- Discovered 3D effects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

Key Impact

- 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)

ALCF Contributions

- Nek5000 has been tuned for the BG architecture in collaboration with ALCF staff over the past few years.



(Right) Duct aspect ratio (width/length) 3 in-plane velocity, streamlines and streamwise velocity. Friction actually increases in this case over square duct cross section due to 3-dimensional effects difficult to measure in experiments.

Discovery and Design of Excited State Phenomena in Next-Generation Energy Conversion Materials

PI: Jeffrey B. Neaton, Lawrence Berkeley National Laboratory

Argonne Leadership Computing Facility

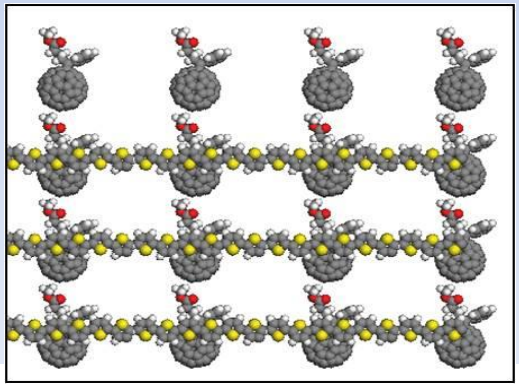
ALCC Award: 23,000,000 hours

Science and Approach

- GW is one of the most accurate methods for computing excited state properties of materials from first principles.
- GW Bethe-Salpeter equation (GW-BSE) calculations are performed on light-harvesting materials to characterize their performance as solar-energy materials.
- These materials are of considerable interest for next-generation photovoltaics and energy conversion applications.

Key Impact

- The largest BerkeleyGW calculations to date (~1000 electrons) were performed on a system resembling realistic interfaces for excitons.
- Computed the first optical absorption spectrum of an organic molecular crystal (TIPS-pentacene) of interest for electronic and solar cell applications.



ALCF Contributions

- ALCF computational resources on Mira are essential for carrying out GW calculations, as implemented in the massively parallel BerkeleyGW code.
- ALCF staff installed and made available input file examples and job submission script for Quantum Espresso (necessary for GW pre-runs).

(Center) PCBM organic donor-acceptor blend currently in use as a component in high-efficiency solar cell.

Argonne NATIONAL LABORATORY

U.S.-Russia Collaboration on Cross Verification and Validation of Thermal Hydraulics Codes

PI: Aleksandr Obabko, Argonne National Laboratory

Argonne Leadership Computing Facility

ALCC Award: 35,000,000 hours (BG/P)
9,000,000 hours (BG/Q)

Science and Approach

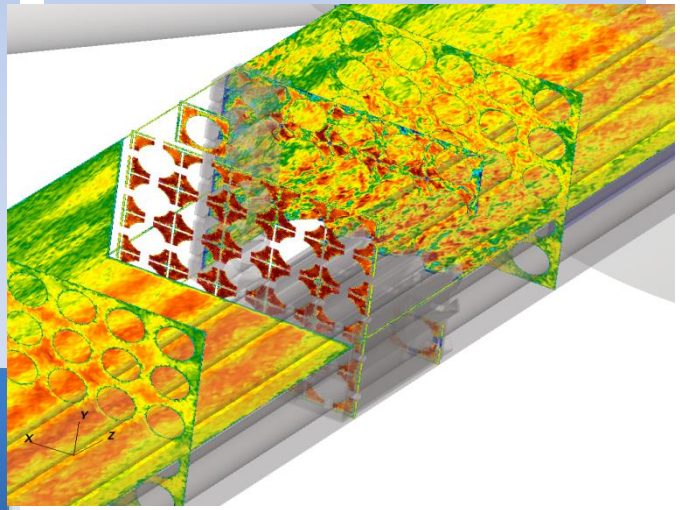
- Collaboration with Russian IBRAE to verify and validate three thermal hydraulics codes for nuclear reactor experiments.
- Nek5000 (ANL), Cfoam-CABARET, and Conv3D Large Eddy Simulation (LES) codes studied.
- Performed LES runs for the OECD/NEA Matis benchmark experiment with larger resolutions of 500 million grid points.

Key Impact

- Validation and verification of codes is important for assessing the prediction capabilities of thermal hydraulics codes for various nuclear reactor applications.
- Improved simulation capabilities lead to safer and more efficient nuclear power.

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.



(Right) Axial velocity for OECD/NEA Matis benchmark. Visualization by A. Obabko, P. Fischer and ANL SHARP team, funded by DOE NEAMS program.

Argonne NATIONAL LABORATORY

Atomistic Simulations of Nanoscale Oxides and Oxide Interfaces

PI: Subramanian Sankaranarayanan, Argonne National Laboratory

Argonne Leadership Computing Facility

ALCC Award: 120,000,000 hours

Science and Approach

- Understand the growth mechanisms and transport phenomena occurring at and across electrochemical interfaces at the atomistic scale.
- Elucidate the process of corrosion initiation and oxide breakdown at the nanoscale.
- Understand dimensionality effects on nanoscale. oxidation and oxide growth.
- Force field-based molecular dynamics (MD) simulations performed with LAMMPS.

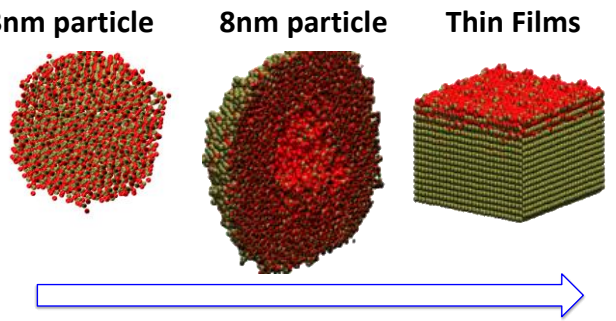
Key Impact

- Our simulations offer a new perspective on the role of solvation dynamics in initiating pitting corrosion.
- Electric field assisted sintering can be used to design oxide materials with controllable composition, microstructure and defect chemistry.
- Simulation results are of great importance to contemporary problems in emerging energy and biomedical technologies.

ALCF Contributions

- Staff, in collaboration with IBM, implemented OpenMP in the REAX-C module of LAMMPS. The time-to-solution was reduced by a factor of two.

Dimensionality effect on oxidation and vacancy formation.



(Right) Large scale reactive molecular dynamics simulations illustrate the dimensionality effect on oxidation and vacancy formation in Fe nanoparticles and thin films. The gas-phase oxygen atoms have been removed for clarity.

Argonne NATIONAL LABORATORY

Dynamics of Conformational Transition in Polymer Grafted Nanoparticles

Argonne Leadership Computing Facility

ALCC Award: 170,000,000 hours

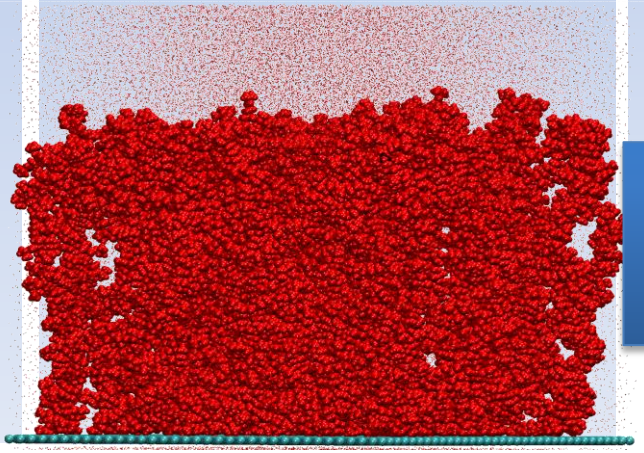
PI: Subramanian Sankaranarayanan, Argonne National Laboratory

Science and Approach

- PNIPAM is a thermosensitive polymer which undergoes a coil-to-globule (CTG) phase transition close to body temperature.
- Molecular dynamic (MD) simulations of PNIPAM-architectures with explicit solvent molecules were performed to study the effect of grafting density on the CTG transition of PNIPAM brush structures.
- Control of temperature dependent phase transitions is important for drug-delivery applications.

Key Impact

- Gained understanding of the role of water in agglomeration and self-assembly.
- Determined that explicit solvent treatment is critical to observing CTG phases transition.
- Determined that grafting density can be used to tune the CTG transition.



(Center) Snapshop of PNIPAM planar structure at 325K from MD simulations

ALCF Contributions

- ALCF staff significantly improved the scaling and performance of NAMD.

Argonne NATIONAL LABORATORY

Chombo-Crunch: Advanced Simulation of Subsurface Flow and Reactive Transport Processes Associated with Carbon Sequestration

Argonne Leadership Computing Facility

ALCC Award: 80,000,000 hours

PI: David Trebotich, Lawrence Berkeley National Laboratory.

Science and Approach

- Establish rules governing emergent behavior at the porous-continuum scale under far-from-equilibrium conditions.
- Careful modeling of the behavior at the underlying pore scale, exploiting new modeling tools.
- Reactive transport modeling at the pore scale, based on direct numerical simulation techniques, is being used to interpret laboratory experiments, with results generalized as a basis for modeling the larger porous-continuum scale.

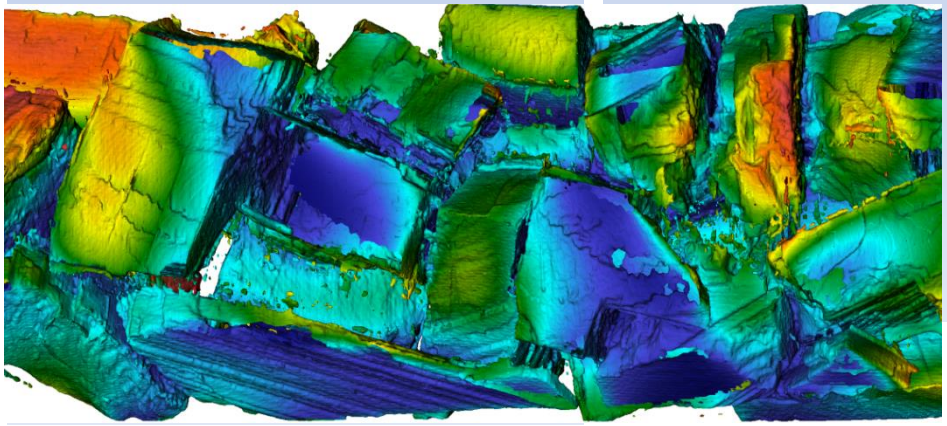
Key Impact

- New phenomenological laws, based on insights gathered from the pore scale investigations, will improve the ability to forecast the fate of CO_2 in actual reservoirs.
- Achieved unprecedented resolution of microscale processes.

ALCF Contributions

- Assisted the project in using the greater memory bandwidth and faster network of Mira to perform deep AMR computations in 3D.

(Right) Capillary tube of 500 micron diameter packed with crushed calcite, embedded boundary representation



Argonne NATIONAL LABORATORY

Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime

Brian Wirth, University of Tennessee

Argonne Leadership Computing Facility

ALCC Award: 7,500,000 hours

Science and Approach

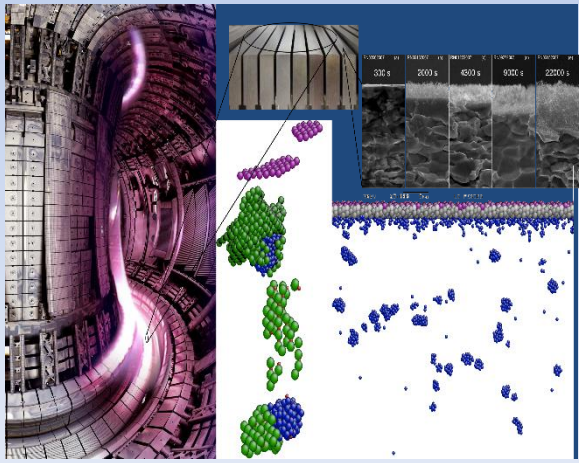
- Large-scale molecular dynamics (MD) simulations for divertor materials on length and time scales relevant to fusion reactors.
- Correlating surface structure of divertor material to sub-surface gas clustering and bubble formation in tungsten exposed to helium (He) plasma.

Key Impact

- Improved knowledge of plasma surface interactions and the materials engineering design of component systems under extreme conditions of a fusion power plant.
- Three invited talks
- *Journal of Applied Physics* **115** (2014) 17351.

ALCF Contributions

- Staff guided users in tuning OpenMP run-time parameter, improving throughput on Mira queues, and improving strong-scaling performance

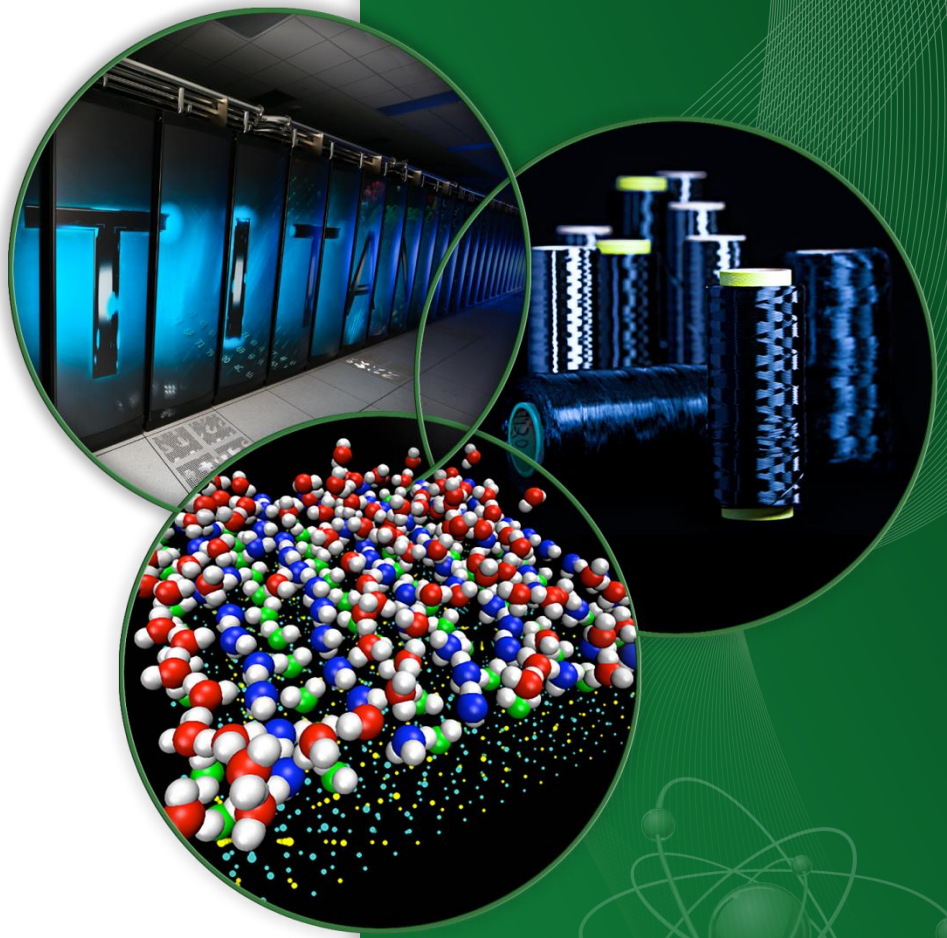


(Right) Composite image showing internal surfaces of tokamak fusion reactor, as well as the castellated tiles of the divertor region which faces severe plasma surface interactions from high fluxes of low-energy helium and hydrogen plasmas. Top right inset shows tungsten surface morphology modiciation observed in linear plasma device exposure to low-energy He plasma. It is now recognized through MD simulations that growing He atom clusters (blue spheres) punch dislocation loops (green spheres) during bubble formation and growth that produce adatom islands (purple spheres) which drive the initial surface roughening leading to nano-scale fuzz formation.

Argonne NATIONAL LABORATORY

OLCF Projects

2013 ALCC

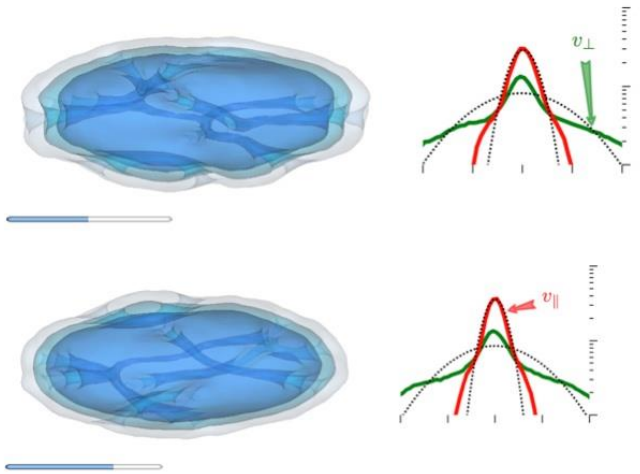


Structure and Dynamics of Nuclear Systems with Time-Dependent Density Functional Theory (TDDFT) Approach

2013-2014 ALCC Project
PI: Aurel Bulgac, Univ of Washington
Allocation: 25M hours
Usage: 26M hours

Science Objectives and Impact

- Apply TDDFT to superfluid systems to study excitation of atomic nuclei and cold atom systems.
- Study the emergence of quantum turbulence in superfluid systems and clarify the nature of experimental observations.
- Produce the first microscopically consistent description of nuclear reactions in medium and heavy nuclei.



Generation of the quantum turbulence and non-equilibrium velocity distribution by crossing and reconnection of quantized vortices in a superfluid, unitary Fermi gas.

Application Performance

- Assisted code conversion from Titan's CPUs to GPUs, resulting in 10x to 25x the performance, with the greatest improvement observed during large simulations.
- Set up a specialized, scalable I/O for advanced checkpoints capable of more than 10 GB/sec.

Science Accomplishments

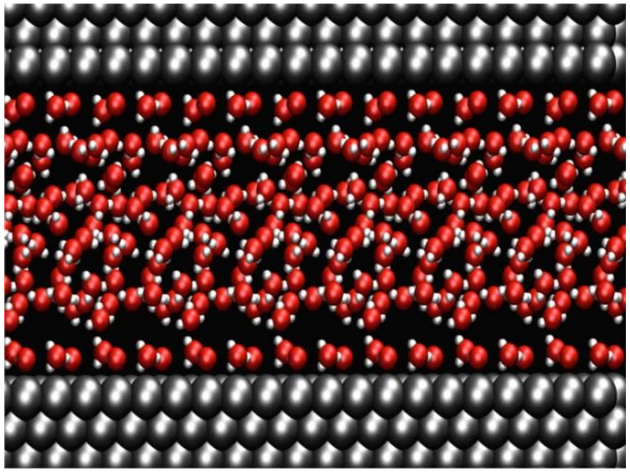
- Completed analysis of the Coulomb excitation of a heavy nucleus by a beam of relativistic uranium nuclei in a first full implementation of TDDFT.
- Simulated within a fully microscopic approach the excitation of quantum vortices in cold atom Fermi gases and demonstrated how quantum turbulence emerges in these systems.
- This data will enable the study of various aspects of nuclear fission, particularly fission fragment distributions.

First Principles Investigations of Adsorbate-Metal Interactions

2013-2014 ALCC Project
PI: Jeff Greeley, Purdue University
Allocation: 25M hours
Usage: 6.4M hours

Science Objectives and Impact

- Leverage new, highly parallelizable quantum Monte Carlo (QMC) and ab initio molecular dynamics (AIMD) codes to explore the interaction of molecules that are central to electrocatalytic reactions and fuel cell science.
- Improve the accuracy of standard Density Functional Theory (DFT) treatments of weak adsorbate-metal bonding and add finite-temperature dynamical effects to the analysis of water-metal interactions.
- Develop highly accurate, fundamental models of electrochemical double layers and study the impact of these structures on electrocatalytic reactions, which are relevant to a broad spectrum of electrochemical phenomena, from fuel cell performance to pollution control.



Ab-initio molecular dynamics simulations of water structure between platinum (111) slabs.

Science Accomplishments

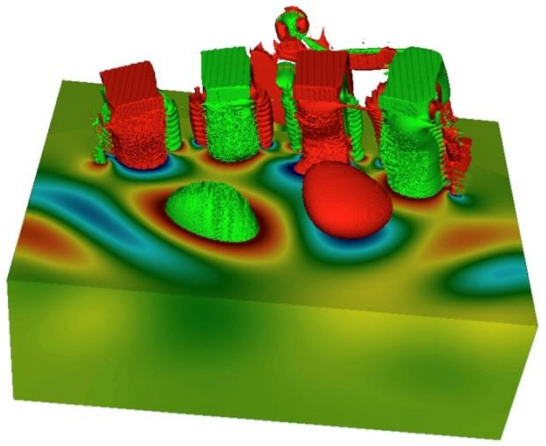
- Resolved a deficiency in “large core” pseudopotentials for platinum that impacts results for calculations on smaller clusters and atoms, expanding the usefulness of QMC calculations for other late transition metals.
- Analyzed the properties of small platinum clusters and determined the equilibrium bond lengths and binding energies of closed shell clusters with a high degree of accuracy.
- For the first time, used QMC-based methods to study the properties of late transition metal surfaces, producing results in agreement with experimental data.

Unraveling the Coupling of Radio Frequency Power to Fusion Plasmas

2013-2014 ALCC Project
PI: David Green, ORNL
Allocation: 50M hours
Usage: 42M hours

Science Objectives and Impact

- Improve understanding of how high-power radio waves can be launched into magnetically confined plasmas for the purpose of nuclear fusion.
- Demonstrate the capability to simulate the fast and slow plasma waves in addition to the sheath potential at the material interface.
- Produce several large data sets for analysis to investigate causes of unexplained power inefficiencies during fusion experiments.



Simulation of the Alcator C-Mod Field Aligned Antenna in pi-mode. The left plot shows fast wave propagation from the antenna for high-edge density. If slow waves are present, their field amplitudes can be high and can contribute to both the amplitude of the radio frequency sheath voltage and to parasitic power losses in the edge plasma.

OLCF Contribution

- Optimized I/O performance by increasing the striping when scaling to more than 100,000 cores.
- Provided resources for simulation requiring more than 1 billion grid cells.
- Supplied data visualization services.

Science Accomplishments

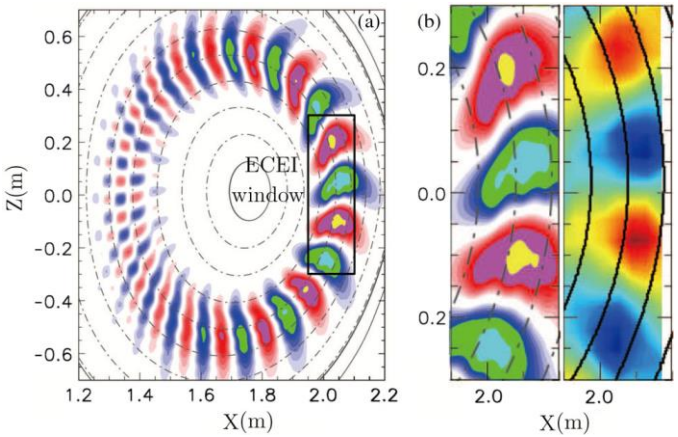
- Produced first high-fidelity 3D simulation of a nuclear fusion experiment with all the relevant physics.
- Simulated fast and slow structures launched by the ion-cyclotron radio frequency antenna and first maps of the radio frequency sheath potentially responsible for plasma impurities.
- The generated data can be examined similarly to experimental data via linear particle tracing for causes behind heating inefficiencies.

Gyrokinetic Simulation of Energetic Particle Turbulence and Transport

2013-2014 ALCC Project
PI: Zhihong Lin,
University of California, Irvine
Total Allocation: 50M
Total Usage: 37.7M

Science Objectives and Impact

- Build predictive capability for energetic particle turbulence and transport in ITER burning plasmas.
- Verification and validation are critical next steps for building the predictive capability of energetic particle confinement in ITER.
- Simulations are part of the SciDAC project, "Gyrokinetic Simulation of Energetic Particle Turbulence and Transport," to support fusion research.



Contour plot of relative electron temperature on a poloidal plane from a GTC simulation. The images are a comparison of structure from the simulation (left) and from the DIII-D experiment (right) in the ECEI window. The red color represents positive perturbations and the blue color represents negative perturbations. *Image credit: Wang, et al. PRL 111, 145003 (2013*)

OLCF Contribution

- Collaborated closely with Scientific Data Group to resolve I/O issue. The Scientific Data Group used its ADIOS middleware to help streamline getting data from the team's GTC code in and out of OLCF computing resources.

Science Accomplishments

- Verified and validated global kinetic simulation as a tool for studying energetic particle turbulence and transport in burning plasmas.
- Found that microscopic kinetic effects profoundly modify the macroscopic magnetohydrodynamic modes.
- Was able to scale simulations to all nodes on Titan, allowing the GTC simulations to incorporate microscopic effects in macroscopic modes.

High-Fidelity Simulations of Transition and Turbulent Separation in Turbomachinery

2013-2014 ALCC Project
PI: Gorazd Medic, UTRC
Allocation: 10M hours
Usage: 15M hours

Science Objectives and Impact

- Assess the use of wall-resolved large-eddy simulation (LES) for predicting details of laminar-to-turbulent transition in the low-pressure-ratio axial fan, turbine first vane, and a turbine stage that includes the effect of stator/rotor interactions.
- Improvements in these turbomachinery components are of key importance in development of UTC's next generation of commercial jet engines that will enable significantly lower fuel burn than traditional designs.

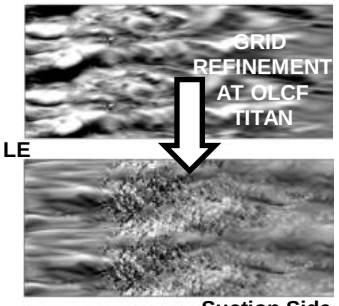
Transition on the suction side of the fan blade at design condition, as predicted with wall-resolved LES. Contours of span-wise velocity at a surface within the boundary layer; strong oscillations indicate the extent of turbulent region.

United Technologies Research Center

Application Performance

Simulations on Titan provide the opportunity to dramatically increase spatial (and temporal) resolution for LES computations – from hundred million to several billions of computational cells.

This, in turn, allows a much more detailed resolution of laminar-to-turbulent transition, as illustrated here for turbine first vane suction side with large inlet disturbances.



Science Accomplishments

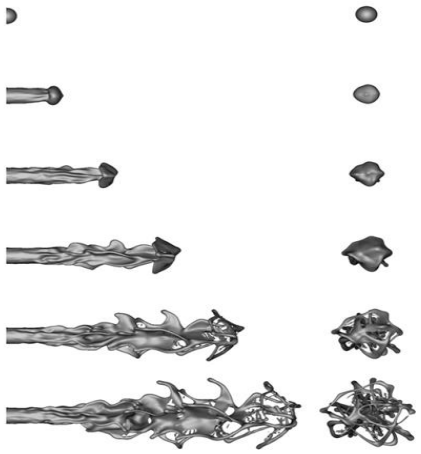
- Demonstrated that wall-resolved LES (at quasi-DNS resolution) is capable of predicting transition locations for turbomachinery flows (in this case for the fan blade). The computed aerodynamic performance agrees well with experimental data.
- First-time demonstration that UTC's in-house LES code can predict transition for 3D turbomachinery configurations.
- Future opportunities for significant improvements in aerodynamic performance of the next-generation of jet engines and an increase in the global market share.

Accelerating Fuel Injector Design

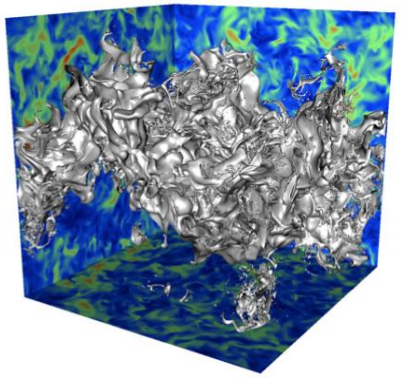
2013-2014 ALCC Project
PI: Madhusudan Pai, GE Global Research
Total Allocation: 46M hours
Total Usage: 54.4M hours

Science Objectives and Impact

- Understand how small changes in complex fuel injector geometries modify spray behavior.
- Employ HPC to understand fuel breakup from first principles.
- Fuel Injectors play a major role in determining engine efficiency, particularly in low emission models. Study shed light on the role of HPC in building next-generation engine architectures with optimized fuel injector designs.



(a)



(b)

(a) Snapshots of EHD enhanced kerosene atomization simulation. Time varies from t=0.0 s (top) to t=0.0005 s (bottom). (b) Topology of liquid gas interface interacting with turbulence.
Image Credit: Oliver Desjardins, Cornell University

Application Performance

- Preliminary simulations indicated a 25 percent speed up of simulations on Titan compared to similar simulations on other commodity clusters.
- NGA code had a 60–75 percent scale-up efficiency on 10–20 thousand compute cores.
- This project resulted in a new algorithm for simulating liquid-gas flows that exhibits better accuracy and conservation properties than existing schemes.

Science Accomplishments

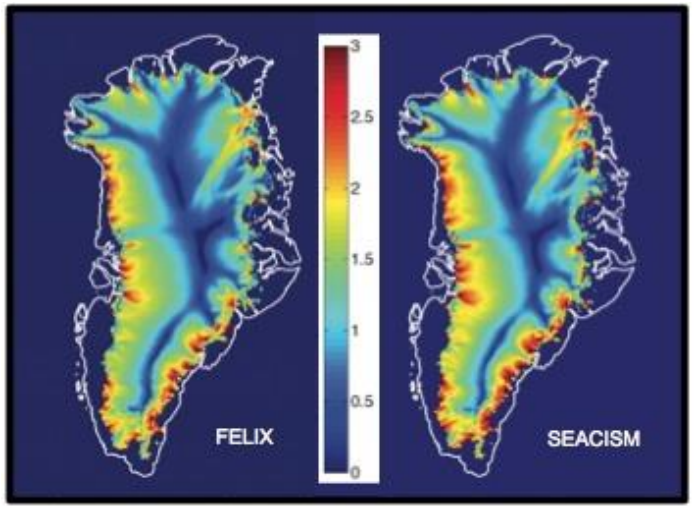
- The first comprehensive simulation of electrohydrodynamic liquid atomization that accounts for electric charge transport within the liquid.
- A new computational database of liquid-gas interface-turbulence interaction that will be exploited to elucidate LES modeling of primary atomization.
- Insights into development needs to perform accurate, robust first-principles simulations of complex fuel injectors.

Projections of Ice Sheet Evolution

2013-2014 ALCC Project
PI: Stephen Price, LANL
Allocation: 2.6M hours
Usage: 2.4M hours

Science Objectives and Impact

- Develop comprehensive verification and validation software for evaluation of ice sheet models.
- Test computational performance of Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES) land ice dynamical cores on large-scale simulations coupled with ice sheet and earth system models.
- Track model performance and fix bugs that adversely affect new ice sheet model, which will enable more accurate projections of future sea level rise due to climate change.



Comparison of simulated Greenland ice sheet surface velocity (log10 [m/yr] scale) using SEACISM dynamical core (right) and prototype FELIX dynamical core (left).

Science Accomplishments

- Profiled performance of new dynamical cores and benchmarked improvements relative to older ones.
- Improved coding efficiency by establishing an automated test suite that regularly confirms the scientific and computational integrity of the ice sheet model during heavy code development.
- Demonstrated Greenland Ice Sheet in high resolution with 1.12 billion degrees of freedom using more than 16,000 processor cores.

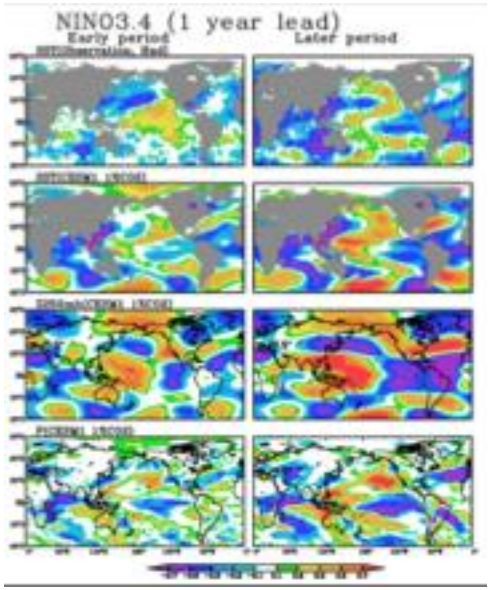
The Role of Aerosols and Multi-Scale Water cycle Processes in Climate Change: Sensitivity to Aerosol Emissions and Modeling Frameworks

2013-2014 ALCC Project
PI: Philip Rasch, PNNL
Total Allocation: 36 M Hours
Total Usage: 44.5 M Hours

Science Objectives and Impact

- Conduct fundamental simulations characterizing uncertainties in climate change projections.
- Investigate the role of aerosols and how their emissions contribute to uncertainties.
- Examine the role of multi-scale water cycle processes and how physics parameterizations, model resolutions, and dynamical frameworks offer additional uncertainties.

Correlation Maps of NINO3.4 Indices with various fields (top to bottom row: observed Sea Surface Temperature (SST), Modeled SST, 250hPA geopotential height, and precipitation). Left column shows the correlation with Pre-Industrial CO2 levels; right column the Present Day Forcing.



Science Accomplishments

- Substantially improved simulations of low clouds by using a high-order turbulence parameterization.
- Established a new experimental strategy for efficient characterization of model sensitivity using CAM5.
- Assessed climate responses to increasing CO_2 via a series of experiments studying precipitation change by perturbing temperature distributions in the tropics and subtropics.

OLCF Contribution

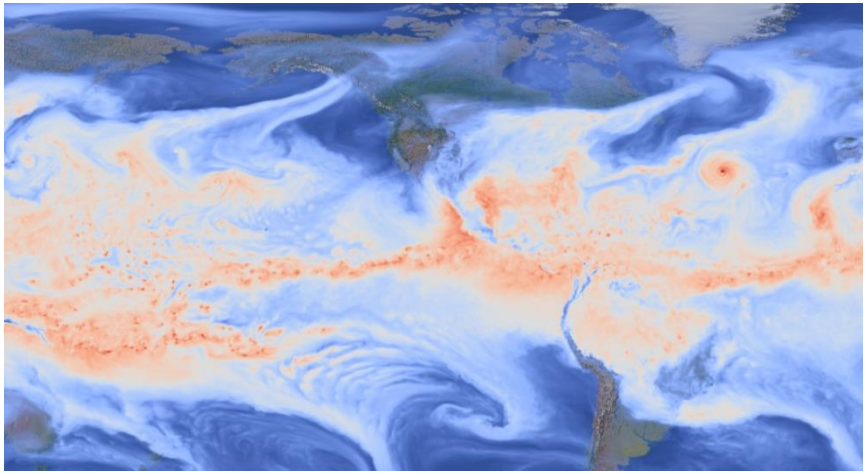
- Provided climate simulations with improved fidelity for the water cycle process.
- Allowed the development of new methods for evaluating and testing climate and weather models.
- Allowed the exploration of new numerical methods for simulating atmospheric dynamics.

High-resolution Coupled Climate Simulations on Titan with GPU Acceleration

2013-2014 ALCC Project
PI: Mark Taylor, Sandia
Allocation: 64M hours
Usage: 68.2M hours

Science Objectives and Impact

- Test the hypothesis that higher resolution climate models are necessary for the accurate and explicit simulation of local to regional scale phenomena, including low-probability, high-impact hydrological events.
- Test the hypothesis that the explicit simulation of non-linear phenomena and small-scale interactions made possible by high resolution climate models has feedbacks on large-scale climate features.



A snapshot of atmospheric precipitable water content simulated by CESM at ¼ degree. At this resolution, CESM can capture tropical cyclones in the mid-Atlantic and other types of severe weather.

Application Performance

- Atmosphere-only climate simulations with full prognostic aerosols ran at an unprecedented 3.4 simulated-years-per-day at weather-resolving resolutions.
- Fully coupled climate simulations, involving atmosphere, ocean, sea ice and land models obtain a throughput of 1.6 simulated years per day using 68K cores.

Science Accomplishments

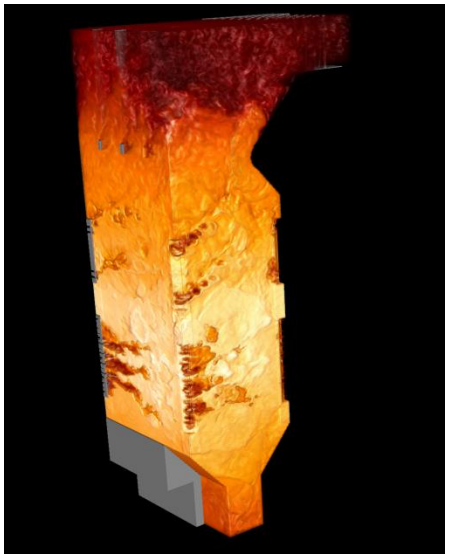
- Tuned first high-resolution version of the CAM5 atmospheric model with prognostic aerosols.
- Tuned for thermodynamic equilibrium, long wave cloud forcing, global aerosol loading and tropical variability.
- Observed reasonable sea ice behavior and ocean sea surface temperature biases during first coupled simulations.
- Documented extreme sensitivity of tropical cyclone formation to the deep convection timescale parameter.

V/UQ Assessment of a Large Eddy Simulation Tool for Clean-Coal Technology

2013-2014 ALCC Project
PI: Jeremy Thornock, University of Utah
Allocation: 7M hours
Usage: 17.4M hours

Science Objectives and Impact

- Produce predictions of heat flux and *O2* concentrations to enable informed decisions regarding operation and new design of industrial coal-fired utility boilers.
- Add a new dimension to the V/Q work performed under the previous 2012-2013 ALCC award.
- Improve computational efficiency through algorithmic and computational infrastructure improvements



Boiler Simulation Facility temperature field demonstrating the gas temperature field from a typical large eddy simulation.

Application Performance

- Arches LES code was made thread-safe, resulting in significant memory savings and load balancing for the boiler simulations.
- The Reverse Monte-Carlo Ray Tracing algorithm was significantly improved for deployment on the GPU.
- The Uintah GPU infrastructure was improved to allow for easier application development and more efficient data handling.

Science Accomplishments

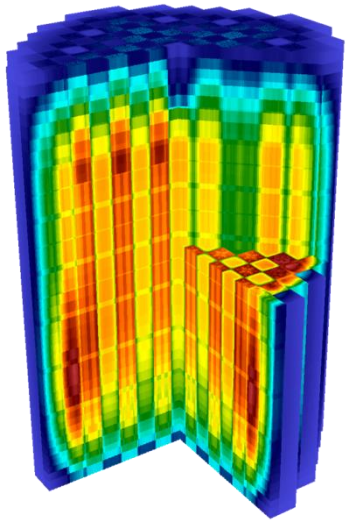
- Higher resolution and new equations governing atmospheric chemistry, biogeochemical processes, and energy absorption and emission will lead to better assessments of regional climate details and predictions of extreme weather statistics.
- CAM5 includes 25 new aerosol calculations affecting modeling of cloud formation, precipitation, and other atmosphere elements, and addresses a key uncertainty on net anthropogenic forcing.

Transforming Modeling and Simulation for Nuclear Energy Applications

2013-2014 ALCC Project
PI: John Turner, ORNL
Allocation: 20M hours
Usage: 64.5M hours

Science Objectives and Impact

- Gain greater insight into light water reactor characteristics.
- Reduce capital and operating costs per unit of energy in light water reactors.
- Reduce nuclear waste volume by enabling higher burnup.
- Enhance nuclear safety by enabling high-fidelity predictive capability for component performance through the onset of failure.



Center for the Advanced Simulation of Lightwater Reactors (CASL) investigators successfully performed full core physics power-up simulations of the Westinghouse AP1000 pressurized water reactor core using their Virtual Environment for Reactor Application code that has been designed on Titan architecture.

Application Performance

- Shift code ran some of the largest Monte Carlo calculations ever performed, consisting of roughly 1 trillion particles.
- Shift was able to scale to 230,000 cores on Titan.
- Denovo code ported to GPUs, ultimately doubling performance.

Science Accomplishments

- Team was able to successfully demonstrate the first large-scale coupled multi-physics model of an operating pressurized water reactor.
- Simulation of Watts Bar Unit 1 Cycle 1 included realistic geometry for fuel, burnable absorbers, spacer grids, nozzles, and core baffle.

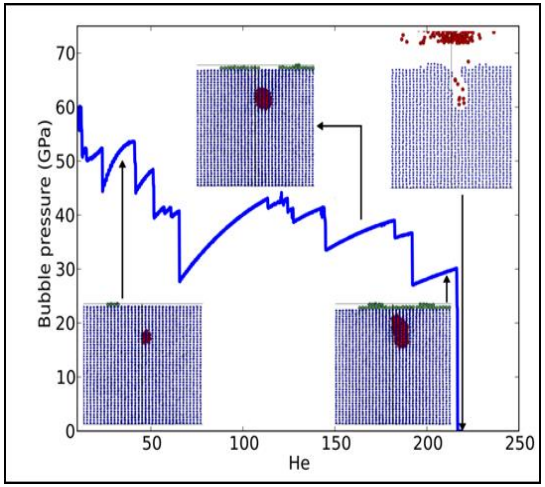
Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime

2013-2014 ALCC
PI: Brian Wirth
University of Tennessee, Knoxville
Allocation: 5M hours
Usage: 9.3M hours

Science Objectives and Impact

- Realizing the promise of fusion energy requires improved knowledge of plasma surface interactions.
- Project aims to evaluate the effect of He gas implantation rate on tungsten surface morphology.
- Develop atomistic database of helium bubble agglomeration kinetics.
- Validate continuum reaction-diffusion models against atomistic simulations.

Bubble pressure as a function of the number of helium added to a growing, sub-surface gas bubble in tungsten, revealing significant pressure drops as the bubble expands through loop punching before eventually bursting and releasing helium.



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 Accomplishments

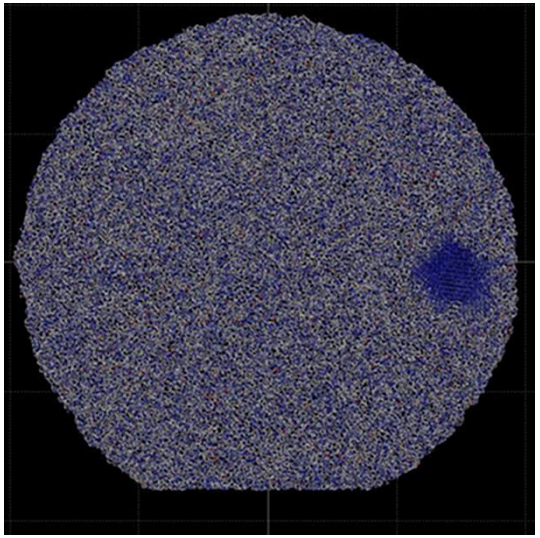
- Parallel replica dynamics reveals the change in bubble growth and morphology as a function of growth rate.
- Accelerated MD simulations performed at the OLCF have confirmed 3 important mechanisms of helium bubble growth:
  - Trap mutation and dislocation loop punching by growing He clusters/bubbles
  - Surface modification by tungsten adatoms/islands of prismatic loops
  - Bubble rupture

Accelerated Modeling of Non-icing Surfaces for Cold Climate Wind Turbines

2013-2014 ALCC Project
PI: Masako Yamada, GE
Allocation: 40M hours
Usage: 53.4M hours

Science Objectives and Impact

- Facilitate the screening of potential anti-icing surfaces by applying the Parallel Replica formalism to molecular dynamics to accelerate the observation of rare freezing events.
- Pinpoint the onset or location of critical nucleus formation during ice accumulation.
- Improve molecular dynamics simulations as a meaningful tool to probe freezing-related phenomena by drastically reducing the time to solution.



Visualization of local water structure near a surface. Blue denotes low mobility molecules, whereas red denotes high mobility ("hot") molecules due to release of latent heat.

Application Performance

- Evaluated strong and weak scaling of the mW water potential with and without GPUs, observing 5x speedup with GPU acceleration for a production droplet.
- Achieved time-acceleration that spanned almost the entirety of Titan using Parallel Replica method, which scales perfectly without code modification.

Science Accomplishments

- Increased project scope to simulate 200 droplets at one time to achieve 100x faster simulations with perfect scaling.
- Observed freezing in all state point, leading to insights on the efficacy of various anti-icing surfaces under a range of conditions.
- As a result of enhanced fidelity simulations, determined the development of anti-icing surfaces must be based on site-specific operating conditions.