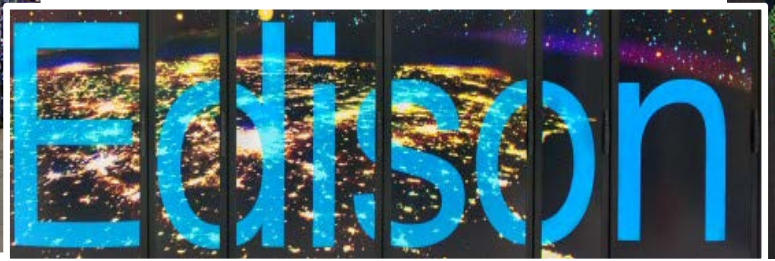
U.S. DEPARTMENT OF ENERGY | Office of Science

ALCC (2012 – 2013)
Project Highlights

OAK RIDGE National Laboratory

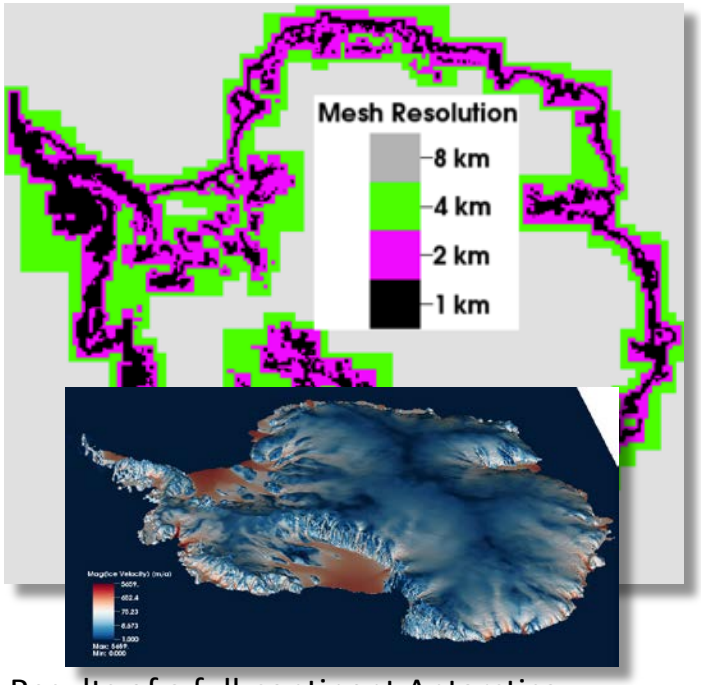
BERKELEY LAB Lawrence Berkeley National Laboratory



Argonne NATIONAL LABORATORY

Projections of Ice Sheet Evolution Using Advanced Ice and Ocean Models

- **Goal: Dramatically improve fidelity of global climate simulation ice sheet modeling; currently a large source of uncertainty in sea level predictions**
- **Completed: New BISICLES code with Adaptive Mesh Refinement allows high spatial resolutions needed for science; implemented an offline-coupling scheme between CISM-BISICLES and the POP2x ocean model**
- **Conducted the first large-scale, coupled ice sheet / ocean evolution simulations for Antarctica and the Southern Ocean; presented in an invited talk at the 2013 AGU meeting**



Results of a full-continent Antarctica simulation at 1-km resolution in equilibrium with initial conditions based on subshelf melt forcing from a POP2x model. Top: Distribution of mesh resolution for this problem. Bottom: Depth-averaged velocity from CISM-BISICLES draped over Antarctic ice sheet surface topography.

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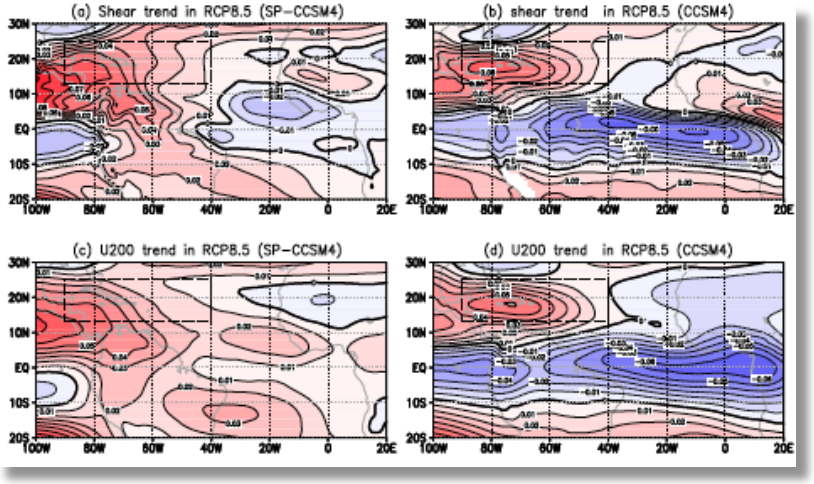
PI: W. Collins, LBNL
Award: 13,000,000 hours

BERKELEY LAB

Reducing Uncertainty of Climate Simulations Using Super-Parameterization (SP)

- **Goal: Determine the effect of an embedded cloud-resolving model that to allows significantly higher cloud resolution on anthropogenic climate change simulations with CCSM4**
- **Completed: Compared response of the tropical Atlantic region to climate change using CCSM with a conventional representation of cloud processes against the SP model; observed a big difference in vertical wind shear and effect of westerly wind jets**
- **Simulation outputs were made available to the atmospheric science community via the NCAR Earth System Grid Gateway**



Computed changes in vertical wind shear; images on the right use superparameterization (SP); those on the right do not.

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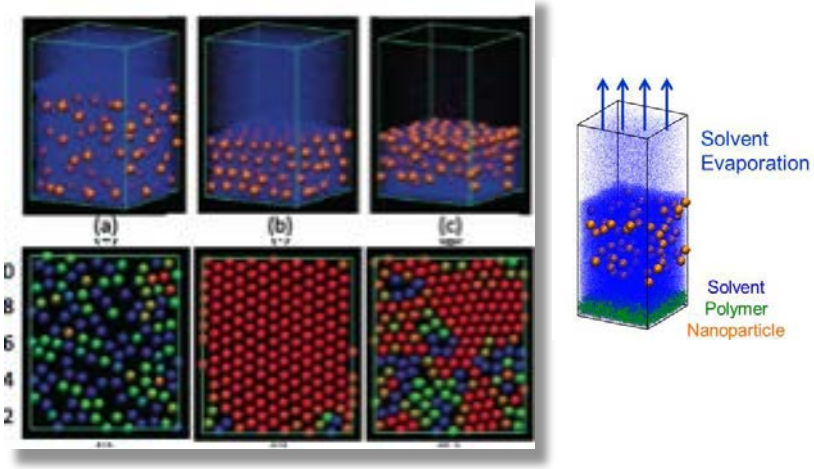
PI: Cristiana Stan, Geo Mason U.
Award: 13,000,000 hours

BERKELEY LAB

Controlling Nanoparticle Interactions to Engineer New Materials

- **Goal: Use simulation to better control self-assembly of nanoparticles to form new devices**
- **Completed: Seven major simulation studies were done, including a study of the diffusion in weakly interacting polymers that have nanoparticles dispersed in them; results conclusively show two very different classes of behavior depending on nanoparticle size.**
- **Others: mechanical strength simulations of polymer composites consisting of end grafted polymers dispersed in a polymer matrix; of evaporation induced assembly of nanoparticles suspended in a polymer/solvent mixture**



Snapshots from simulation of solvent evaporation; solvent shown in blue; time increasing from l to r; top is side view, bottom is top view. These results were selected for the cover of the Journal of Chemical Physics, February 8, 2013

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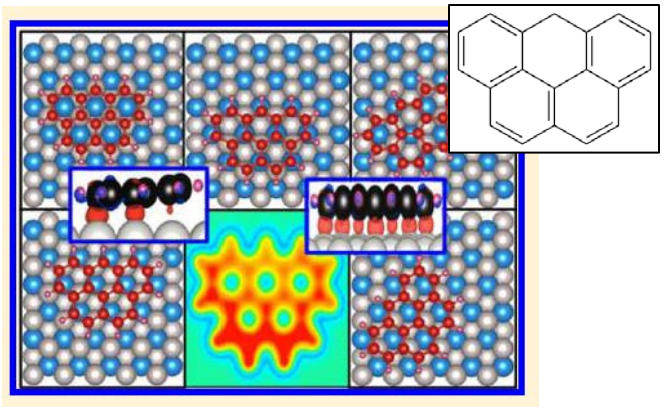
PI: G. Grest, Sandia Nat'l Labs

Award: 30,000,000 hours

BERKELEY LAB

Computational High-Throughput Screening of Organic Materials for Solar Energy and Lighting

- **Goal: Explain the electronic structure of the interface between organic molecules and metal surfaces to help design light-weight, flexible, low-cost, and durable electronic devices.**
- **Completed: Studied adsorption of the "Olympicene" molecule on copper to explain characteristics of metal-to-carbon bonding that takes place – bonding that represents a unique transition between physical adhesion and true chemical bonding.**
- **Three papers already published; five will be submitted within the next few months.**



Olympicene is an organic molecule consisting of five fused rings in the shape of the Olympics emblem that has promising electronic and optical properties. The image shows various views from a simulation study of the molecule adsorbed on a surface of copper atoms.

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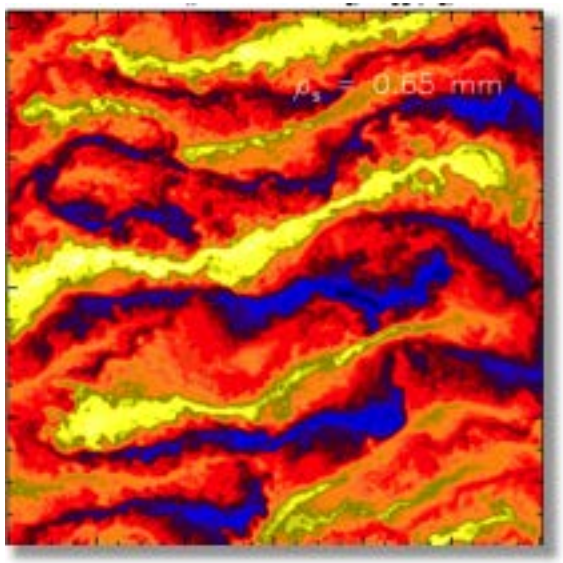
PI: AbdelKader Kara, U. Central Fl.
Award: 6,000,000 hours

BERKELEY LAB

Gyrokinetic Simulations of Multiscale Electron Turbulence for Improved Tokamak Plasma Modeling

- **Goal: Use the highly mature and well-verified GYRO code for high-resolution multiscale gyrokinetic simulations of electron turbulence in current tokamaks to predict performance of future experiments such as ITER.**
- **Completed: Physically-comprehensive simulations show that for some plasma discharges, ion gyroradius scale models underpredict electron thermal transport and that electron turbulence effects account for the difference between ion-scale models and experimental values.**
- **Three papers published, one submitted, and one more in preparation.**



Visualization of small-scale electron temperature fluctuations in the Alcator C-mod tokamak. Note that as the ion sound gyroradius ρs = cs/Ωci = 0.65 mm in this plasma, the visualization corresponds to a physical domain of approximately 8 mm x 5 mm.

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PI: Chris Holland, UCSD

Award: 30,000,000 hours

BERKELEY LAB

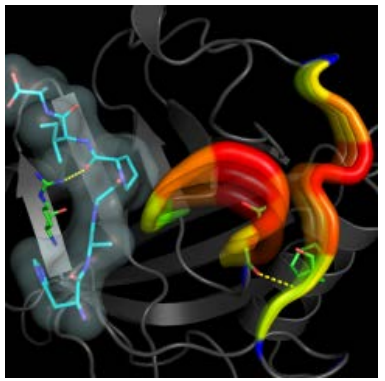
Understanding the Factors that Affect the Efficiency of Bio-Catalytic Processes

Pratul Agarwal, ORNL
Award: 5,000,000 hours

OLCF
Oak Ridge Leadership Computing Facility

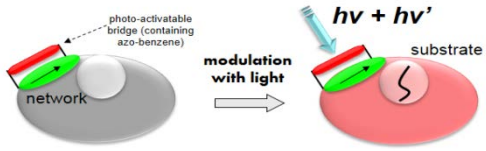
Science Objectives and Impact

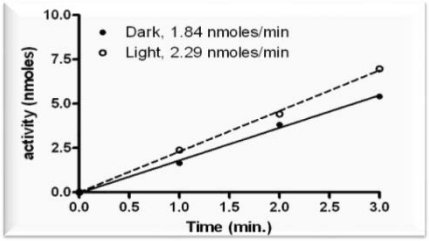
- Develop a hyper-catalytic enzyme engineering approach, which allows over 100 fold improvement in enzyme activity.
- Understand the inter-connection between enzyme structure, dynamics and catalysis.
- Identify enzyme catalysis promoting conformational fluctuations and conformational sub-states.
- Impact: Highly efficient enzymes enable cheaper and faster industrial processes.
- Application: Hyper-active cellulases will allow renewable cellulosic bio-ethanol.



Over 15 publications including the covers of following journals:
• *J. Phys. Chem. B* (2009), 113 (52), *J. Phys. Chem. B* (2011), 115 (28) and *PLoS Biology* (2011), 9 (11)
• 1 US patent granted: Identification and Modification of Dynamically Active Protein Residues # *8,417,461*

Science Breakthrough





Hyper-catalytic enzyme developed: *30X improvement over wild type*

Science Results

- Identified and characterized the role of reaction promoting dynamics in enzymes including: cyclophilin A, dihydrofolate reductase, ribonuclease A, lipase B from *C. antartica*.
- *Discovered that the reaction promoting dynamics is a conserved part of the enzyme fold.* Enzymes structures with low sequence identify from bacteria to human show conserved dynamics
- Developed and tested a hyper-catalytic enzyme engineering approach: *>30X improvement in the activity of enzyme lipase B** achieved through a novel approach of conformational modulation

* Agarwal et al., *J. Phys. Chem. Lett.* (2012), 3, 1142-1146.

OAK RIDGE National Laboratory

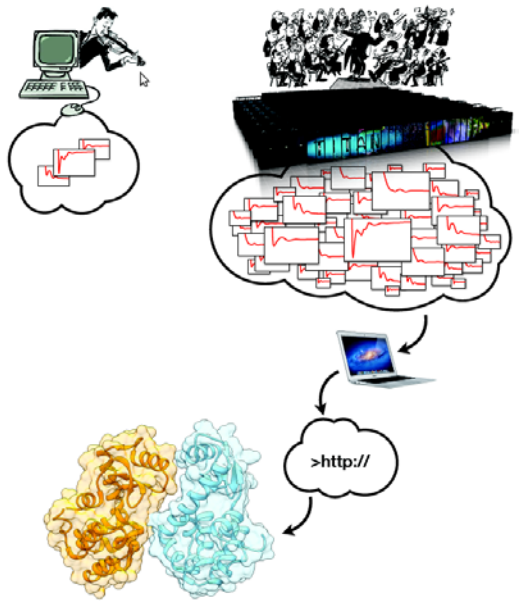
Protein Folding and Computational Models

Ken Dill, Stony Brook Univ
Award: 2,000,000 hours

OLCF
Oak Ridge Leadership Computing Facility

Science Objectives and Impact

- Use the capability of Titan to explore in detail how water behaves in the neighborhood of a systematic series of solutes of increasing size and electrostatic interaction magnitude.
- Develop an accurate set of effective interactions that can be instantly assigned to any given molecular system without need for pre-simulations.
- This information is useful in building accurate, effective solation interactions of more complex biomolecules. It helps to reduce the computational cost of numerical simulations of bigger systems.



Effective interaction solvation information flow: Titan supercomputer enables one to uncover fundamental tendencies for microscopic solvation perturbation across systematic series of solutes. This information can be used next to simulate much more complex biomolecular systems on computers with a fraction of the available horse-power. Simple web-lookups can be built to generate unique, effective interactions for one's specific system of interest.

OLCF Contribution

- Use of the Lens analysis and visualization cluster was essential for setup and analysis of our Titan simulations. Without Lens, it would have been exceedingly difficult to get this project started.
- OLCF user support acted as a liaison between our scientific efforts and job execution on the Titan cluster. Furthermore, OLCF user support identified limitations in the parallel nature of our effort and set into motion improvements to counteract these limitations, which increased the usability of Titan for future research.
- Titan enabled us to break up tedious simulations into hundreds of shorter ensamble fragments and accomplished overnight what would normally take us several months.

Science Results

- Tetrahedral order parameter of water molecules as a function of solute proximity was determined for simple hydrophobic and charged solutes. A significant sampling of slovent configurations was performed to get converged values.
- This information enabled us to better understand the degree by which a certain solute affects the hydrogen-bonding network of water around a given solute.
- An extensive grid of various solute-solute potentials of mean force (PMFs) was built and used for predicting PMFs without running extensive simulations (we need few seconds to compute the entire PMF).
- We can predict, for example, constants of hydrophobe association or ion pairing with negligible computational cost.

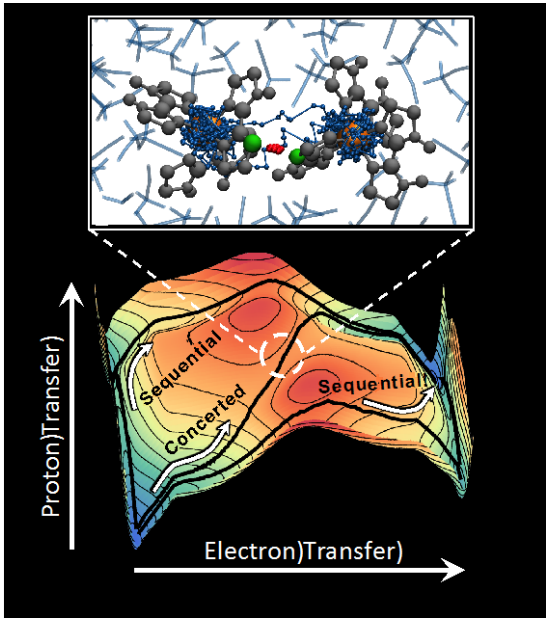
OAK RIDGE National Laboratory

Coupled Electronic and Nuclear Dynamics in Solar Photocatalytic Water Splitting

Thomas Miller, Caltech
Award: 5,000,000 hours

Science Objectives and Impact

- Perform direct simulations of proton-coupled electron transfer (PCET) reactions in prototypical inorganic catalysts and photocatalysts
- Understand the mechanistic features and driving forces for PCET reactions under diverse conditions
- Yield insights into PCET reactions that are fundamental to energy storage and conversion
- Demonstrate powerful new theoretical methods to understand, predict, and control the reactivity and flow of energy in molecules and materials



This image shows competing sequential and concerted pathways for the PCET reaction in a symmetric iron bi-imidizole complex, with the reaction pathways overlaid on the energy landscape for the system in the ET and PT coordinates. Above, the image shows a snapshot of the molecular complex during concerted PCET, which illustrates the partially transferred electron (blue) and the partially transferred proton (red) in the ring-polymer molecular dynamics (RPMD) representation.

OLCF Contribution

- Sampled real-time quantum dynamical trajectories for PCET reactions in systems with up to 5000 atoms
- Performed extensive free energy sampling for these systems, requiring up to 20,000 cores.

J.J. Warren, et al., J. Phys. Chem. Lett., (2013).
J.S. Kretchmer and T.F. Miller, J. Chem. Phys., (2013).
A.R. Menzeleev, et al., in prep., (2013).
J.S. Kretchmer, et al., in prep., (2013).

Science Results

- Revealed kinetics and mechanistic features of concerted PCET reactions across multiple coupling regimes, spanning from weak to strong coupling for both the electron and proton.
- Discovered a new “transient-proton-bridge” mechanism for concerted PCET in the transition between the superexchange mechanism for fully non-adiabatic PCET and the hydrogen atom transfer mechanism for partially adiabatic PCET.
- Explained recent experimental results by demonstrating that conformational fluctuations in molecular catalysts can give rise to anomalous PCET reaction rates.

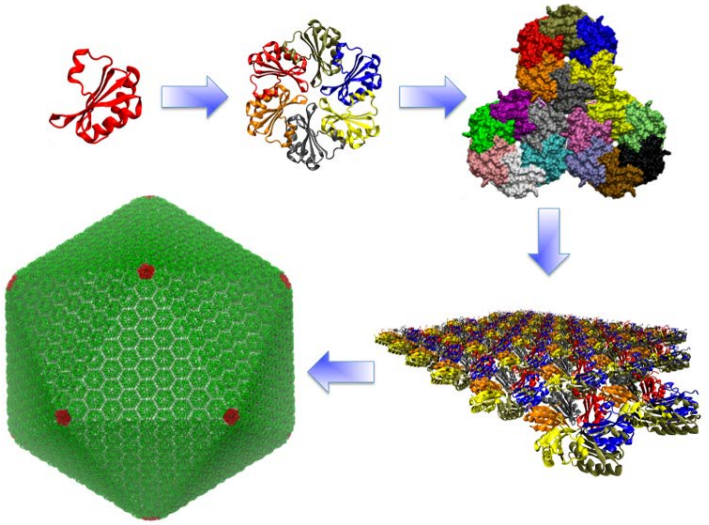
Multiscale Reactive Modeling of Carboxysomes

Gregory A. Voth, U. Chicago/ANL
Award: 8,000,000 hours

OLCF
Oak Ridge Leadership Computing Facility

Science Objectives and Impact

- To better understand the complex process by which bacteria sequesters CO_2 and efficiently transforms this greenhouse gas into useful energy.
- A detailed molecular understanding of the entire process will guide the engineering of future clean energy technologies.
- To develop physically grounded multiscale models of a complete multi-protein carboxysome shell and constituent enzymes.
- To design computationally efficient algorithms to model reactive processes.



Construction of the carboxysome shell structure from the basic protein building blocks.

OLCF Contribution

- Computing resources afforded converged simulations of required large-scale atomistic systems with practical time to solutions.
- Large-scale GPU resources and local expertise to facilitate testing and benchmarking of new simulation algorithms.

Science Results

- Atomistic simulations of carboxysome walls form the basis of coarse-grained models for full-scale simulations.
- Results from equilibrium simulations of several key enzymes used to guide development and validate multistate reactive models.
- Implementation of GPU algorithms to accelerate computation of reactive multistate simulations appropriate for condensed phase systems.

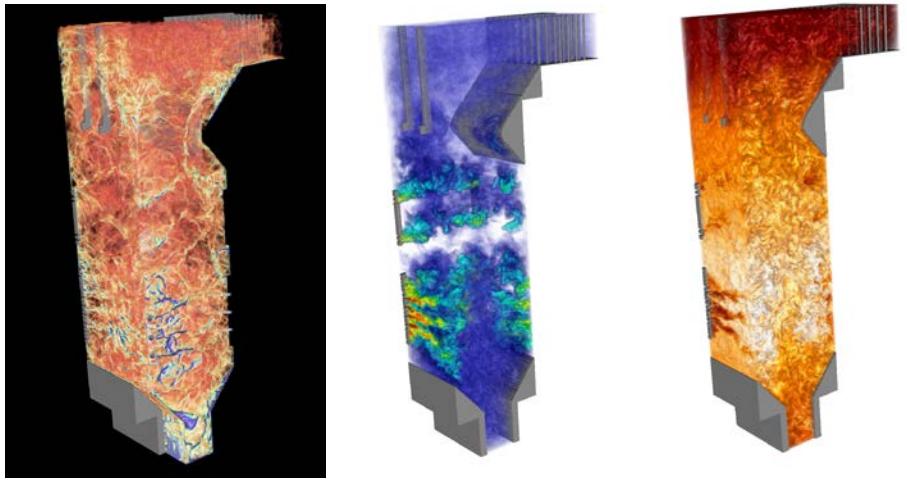
OAK RIDGE National Laboratory

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

Jeremy Thornock, Univ of Utah
Award: 20,000,000 hours

Science Objectives and Impact

- Demonstrate LES predictability for oxy-coal applications using a data-collaboration approach for assessing simulation uncertainty.
- Provide a predictive tool for modern boiler design and retrofit applications with quantified uncertainty.
- Advance the heterogeneous scaling capabilities of the Uintah Computational Framework and the Arches LES component.
- Bring high-fidelity simulation to an applied combustion problem in industry.



Images (from left to right) of large coal particle distribution, oxygen concentration, and temperature throughout the boiler.

OLCF Contribution

- ~15M CPU hours on Titan for performing several full-scale boiler simulations, varying several input parameters over their uncertainty ranges.
- ~2M CPU hours on Titan for performing testing of NOx formation model on a full-scale industrial steam-generator.
- ~3M CPU hours on Titan for performing scaling tests, CS advances and finer mesh resolution demonstration of the boiler.
- Use of LENS for visualization of results using the VisIt software package.

Science Results

- First-ever full boiler scale simulation using high-fidelity LES
- Initial validation of the LES results with experimentally measured data
- Performance advancement (factor of 2) for the LES capability
- First-cut demonstration of the GPU implementation of reverse Monte-Carlo for performing radiation calculations
- Scaling demonstration of the Uintah hybrid scheduler
- GPU implementation of key pieces of the DQMOM solution process

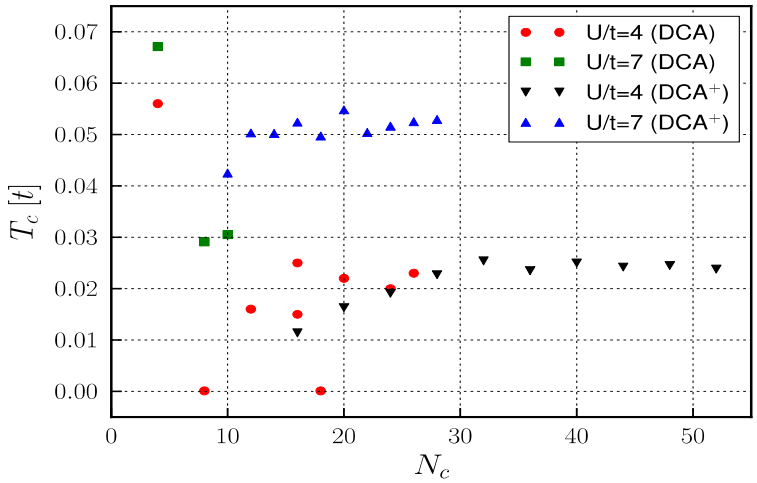
Predictive Simulations of Cuprate High-Temperature Superconductors

Thomas Maier, ORNL
Award: 50,000,000 hours

OLCF
Oak Ridge Leadership Computing Facility

Science Objectives and Impact

- Long-term goal: Understand the mechanism underlying unconventional superconductivity in the cuprate high-temperature superconductors.
- Understand the factors, which determine the transition temperature and their variation between different cuprates.
- Superconducting materials are key components to developing new energy related technologies, but require optimization to unleash their full potential. Understanding and predicting their behavior through high-end computation will help accelerate development in this area.



The new DCA+ algorithm provides converged results in cluster size Nc for the superconducting transition temperature Tc for the weakly interacting (U/t=4) and strongly interacting (U/t=7) regimes of the 2D Hubbard model of the cuprate superconductors.

OLCF Contribution

- Extensive use of OLCF Compute Resources (Titan).
- The OLCF team worked closely to provide timely access and throughput for full scale SC 13 Gordon Bell runs.

Science Results

- Cluster size dependence of the pseudogap temperature, below which low-energy electronic spectral weight is reduced, indicates that pseudogap arises from short-range correlations.
- Evidence that superconductivity at 125 K arises from repulsive interactions in the 2D single-band Hubbard model with realistic parameters relevant for the cuprates.
- Supercomputing 2013 Gordon Bell finalist for dynamical cluster approximation (DCA+) that simulates a cluster of atoms using the Hubbard model.

OAK RIDGE National Laboratory

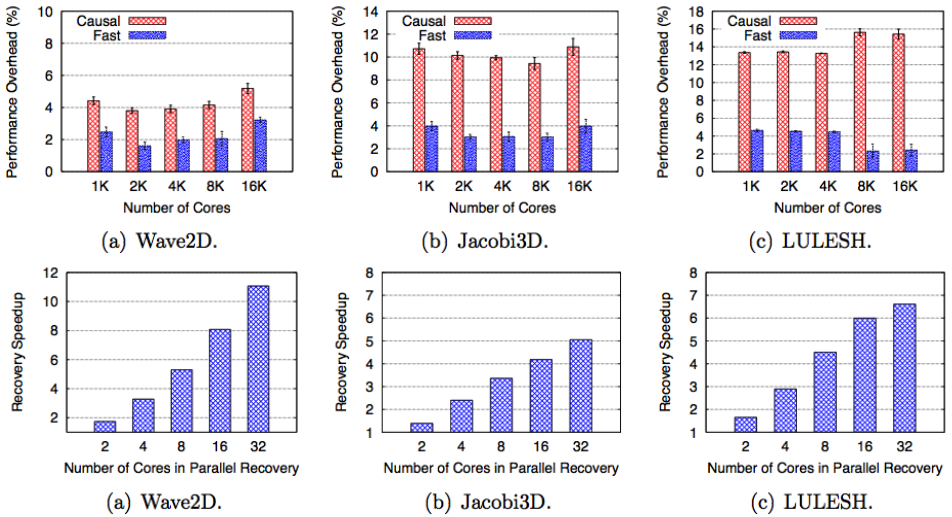
HPC Colony: Adaptive System Software for Improved Resiliency and Performance

Terry Jones, ORNL
Award: 3,000,000 hours

OLCF
Oak Ridge Leadership Computing Facility

Science Objectives and Impact

- As supercomputers grow in component count and overall complexity, the hardware interruptions experienced by applications will be key.
- Supercomputers rely on a technique called checkpointing to provide fault tolerance. Checkpointing consists of storing a snapshot of the current application state, and later on, using it for restarting the execution in case of failure. However, checkpointing has critical scaling issues.



A new checkpoint scheme that avoids the use of "determinants" (top graph) and incorporates parallelism (bottom graph) improves application performance.

OLCF Contribution

- Utilized over 3M core-hours on Titan
- Geographically distributed team worked with OLCF's User Services to obtain assistance with accounts and access.
- Utilized Titan programming environment to develop new system software

Science Results

- Through incorporating improved checkpointing schemes into an intelligent runtime system, programs can now be restarted with lower overhead.
- Impact applies to wall-clock turnaround as well as energy savings.
- These results were incorporated into the PhD thesis of Esteban Meneses and are publically available through the library system of the University of Illinois.

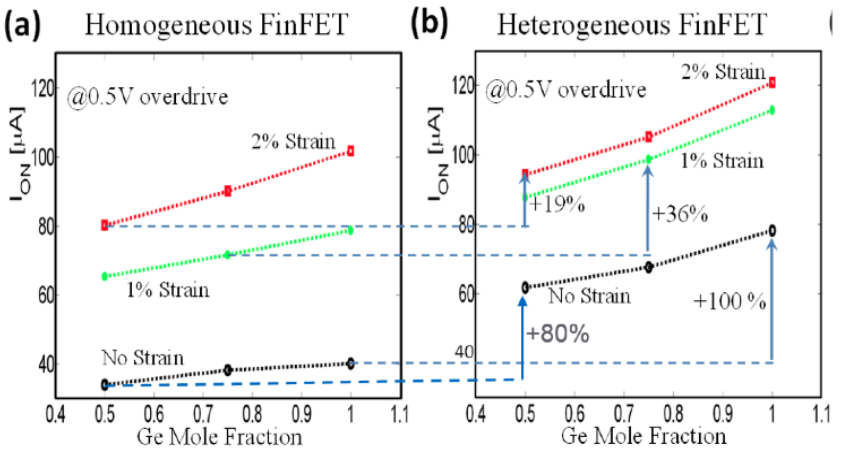
OAK RIDGE National Laboratory

Semiconductor Electronics Atomistic Simulations of Ultra Scaled Transistor

Behtash Behin-Aein
GLOBALFOUNDRIES
Award: 8,000,000 hours

Science Objectives and Impact

- Determine if SiGe is a good substitute for Si in PMOS transistors.
- For properly designed devices, SiGe PMOS transistors can significantly outperform their Si counterparts.
- Heterogeneous devices are in fact feasible since the transport carriers can be confined in a narrow (2-3 nm) clad region.
- Given the very high cost of transistor scaling and also performing many wafer experimentation, the possible design parameters space has been significantly reduced.



Calculated overdrive current for (a) homogeneous FinFET and (b) heterogeneous FinFET with 3 nm clad width with different Ge mole fraction and strain.

OLCF Contribution

- OLCF system runs very smoothly and the software gives proper feedback on the simulations that are unsuccessful.
- Application performance is extremely high running on the systems
- OLCF user assistance center support has been particularly helpful.

Science Results

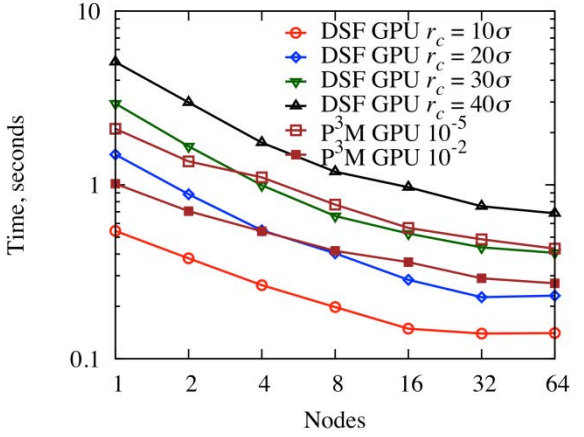
- A thin SiGe cladding layer can confine a significant ratio of overall carriers in a heterogeneous structure.
- While only 3nm thin, the cladding layer can carry a large current and the overall device performance is much better for heterogeneous structures rather than homogeneous structures.
- Quantum confinement enhances transport in the <110> direction.

Computational Partnerships:
The OLCF ARRA-funded post-doctoral program

B. Messer & J. Hill, ORNL
Award: 25,000,000 hours

Objectives and Impact

- The Computational Partnership Postdoctoral program at the OLCF was funded by the DOE/ASCR office with funds from the American Recovery and Reinvestment Act of 2009.
  - Funded expressly with the purpose of fostering innovation in computational science across a wide range of application domains
  - To make significant contributions to their respective domain areas, postdocs required access to the world-class computational facilities available at the OLCF.
  - Post-doctoral associates were mentored by OLCF computational scientists.



Advanced models for electrostatic interactions in bottle-brush systems (left). Strong scaling performance of the damped shifted force (DSF) model and of the particle-particle particle-mesh (P3M) model on the ORNL Titan supercomputer with GPU acceleration (right). For further information, see Nguyen, et. al. , J. Chem. Theory Comput (2013)

OLCF Contribution

- 25M Titan core-hours were awarded and consumed by five post-doctoral associates in the 2012-2103 ALCC year
- Continued access to OLCF resources through a Director's Discretionary allocation is enabling ongoing analysis of simulation results.

Science Results

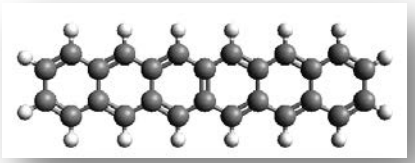
- Resulted in eleven refereed journal publications either accepted or published and seven conference or workshop presentations in applications areas ranging from astrophysics to materials science.
- Algorithmic contributions to two production software applications (LAMMPS, WL-LSMS) that have been or will be rolled into the publicly released versions.

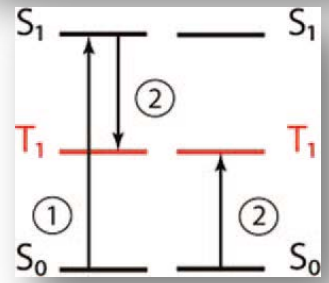
High-Level Studies of Excited States in Light Harvesting Systems and Complex Emergent Phenomena

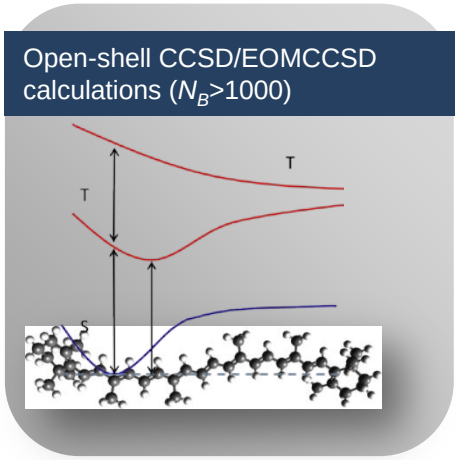
Karol Kowalski, PNNL
Award: 5,000,000 hours

Science Objectives and Impact

- The primary goal of this research was to study new types of light harvesting processes with equation-of-motion coupled cluster methods and multi-reference coupled-cluster approaches.
- The secondary goal was to enable high level methods capable of describing correlation effects in highly correlated systems.
- Study complicated excited states dominated by double excitations in systems revealing singlet fission behavior (pentacene, β-carotene).
- Understand triply excited states in the components of singlet fission systems.







Excited states relevant to the singlet fission processes have been studied for pentacene and β-carotene molecules using MRCC and EOMCC formalisms.

OLCF Contribution

- Enabling MRCCSD(T) calculations for the pentacene system
- Providing an opportunity for testing GPU implementation of the MRCCSD(T) formalism
- Preliminary tests indicate 5-6 time speedup of the GPU implementations of the non-iterative methods compared to the CPU-based runs.

Science Results

- The large-scale calculations using MR-CCSD(T) approach predict hat the excitation energy for doubly excited pentacene is 0.5 eV higher than the results obtained with multi-reference perturbation theory. These results demonstrate the role of individual correlation effects needed to describe excited states.
- In the largest up-to-date CCSD/EOMCCSD calculations for the triplet excited states in β-carotene (both vertical and adiabatic excitations) we showed that β-carotene satisfies the excitation energy balance between doubly excited singlet and triplet states. This is a prerequisite for efficient singlet fission.
- B.N. Kiran, *et al.* Noniterative Multireference Coupled Cluster Methods on Heterogeneous CPU−GPU Systems. J Chem Theory Comp. (2012)

Gas Turbine Combustor

Analysis of a multi-cup GE Gas Turbine Combustion using Large Eddy Simulations

Anne Dord, GE
Award: 34,000,000 hours

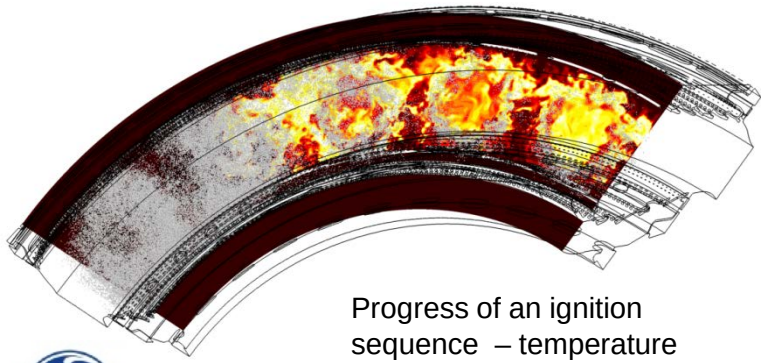
OLCF
OAK RIDGE LEADERSHIP COMPUTING FACILITY

Science Objectives and Impact

Science objectives

- Understand the impact of side walls on flow distribution in center cup
- Understand the impact of cup to cup fuel variation on exit temperature distribution
- Demonstrate ability to run combustor engine geometries at scale

Impact: Being able to study parametric variation at that scale is a first step towards the understanding of nozzle to nozzle coupling in gas turbines. This opens new areas for flow optimization.



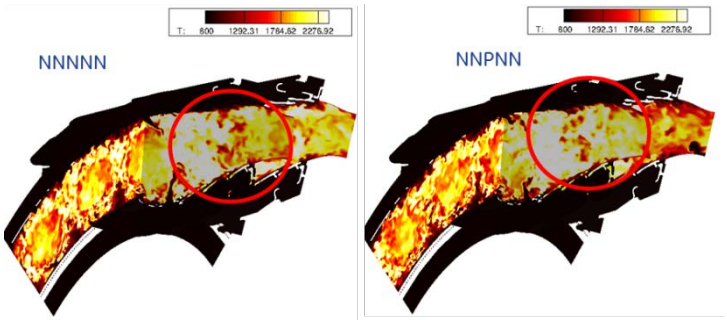
Progress of an ignition sequence – temperature contours and discrete fuel droplets

Application Performance

- All simulations performed using the Cascade Technologies Vida flow solver
- 72 h / Flow Through Time using 20 k cores

Science Results

- Unprecedented detail and accuracy of a CFM56 engine simulation
- First circumferential tolerance effect study – demonstrated potential for future design optimization



Instantaneous temperature distribution

'Now we can estimate the effects of tolerances on key combustor exit parameters'
Narendra Joshi, Chief Engineer, Advanced Technology Leader GE Global Research

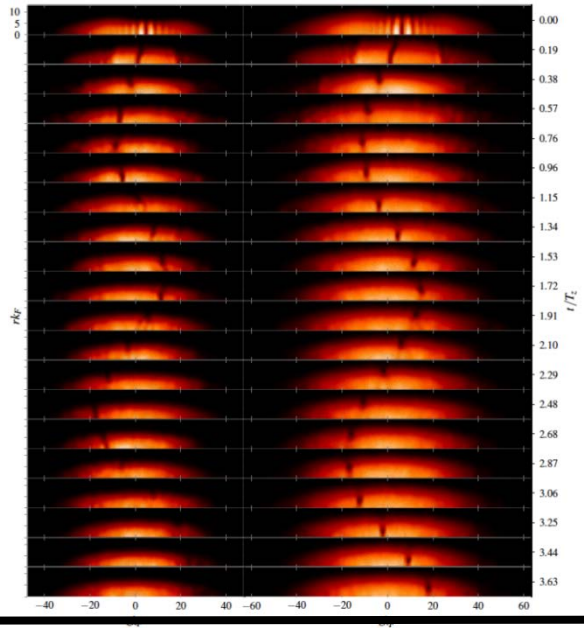
OAK RIDGE National Laboratory

Time-Dependent Density Functional Theory (TDDFT) Approach to Nuclear Reaction

Aurel Bulgac, Univ of Washington
Award: 12,000,000 hours

Science Objectives and Impact

- We have combined the latest developments in DFT (Density Functional Theory), the (TD)SLDA ((Time-Dependent) Superfluid Local Density Approximation), with the best computer science methods for leadership class computers.
- We will use our software to describe nuclear structure, nuclear reactions and ultimately induced fission in a unified formalism within appropriate validated extensions of the DFT applied to nuclear systems.
- This major theoretical advance will lead, for the first time, to a microscopically consistent description of nuclear reactions in medium and heavy nuclei.



Oscillations of a vortex ring in a vortex ring in a 24 24 96 lattice (left) and a 32 32 128 lattice (right)

OLCF Contribution

- We have implemented GPUs in our simulations and obtained significant speed-ups of the code.
- Using GPUs we were able to simulate the dynamics of a cloud of cold atoms and simulate a recent experiment.

Science Results

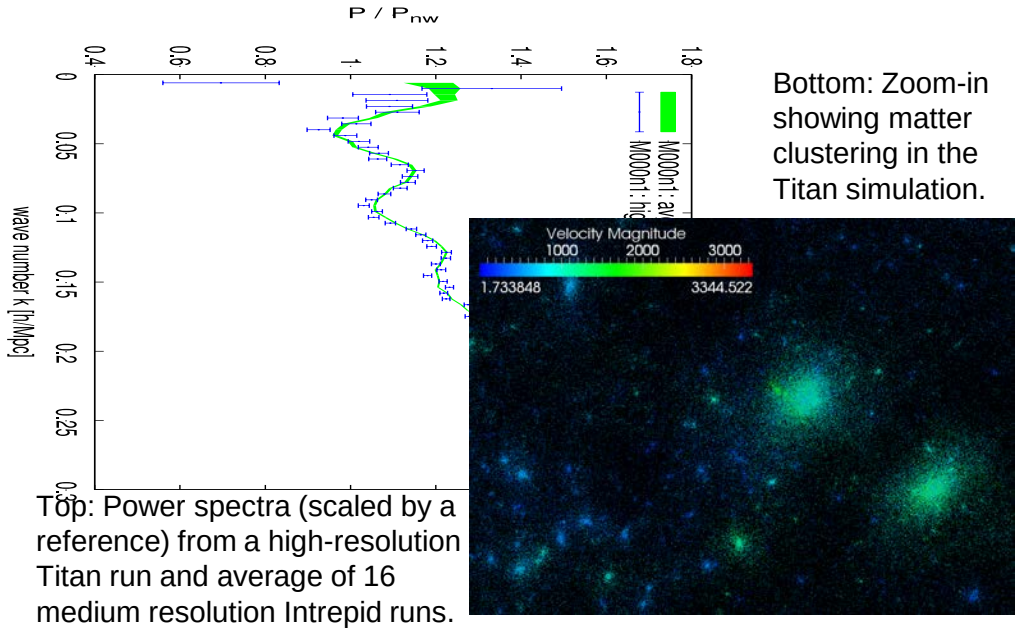
- During the entire allocation period we increased the accuracy of the code and performed a number of improvements.
- We constructed a new ground state solution for ^{238}U with a smaller lattice constant of 1 fm and on a larger simulation box of 40^3 fm^3.
- We have developed a new theoretical framework to analyze the results of Coulomb excitation and have obtained an accurate estimate of the emitted protons and neutrons and the total excitation energy of the target nucleus.
- Publication: G. Wlazlowski, P. Magierski, A. Bulgac, and K.J. Roche, Phys. Rev. A 88, 013639 (2013)

Exploring the Nature of the Lightest Massive Particles in the Universe

Katrin Heitmann, ANL
Award: 6,000,000 hours

Science Objectives and Impact

- Future cosmological measurements will be sensitive to the combined effects of dynamical dark energy and massive neutrinos
- Precision simulations including these effects are crucial to extract this information from observations
- Large mass difference between dark matter and neutrino tracer particles poses numerical challenges for a two-species method
- Here: Follow approximate approach, show that it is accurate at the ~1-2% level, investigate effects of neutrinos and dynamical dark energy on cosmological measurements



Bottom: Zoom-in showing matter clustering in the Titan simulation.

Top: Power spectra (scaled by a reference) from a high-resolution Titan run and average of 16 medium resolution Intrepid runs.

OLCF Contribution

- Large allocation on Titan to carry out state-of-the-art simulations
- Support for fast turn-around of very large scaling runs
- Without major optimization of the GPU force kernel, we achieved roughly a factor of 10 speed-up using Titan compared to the CPU version.
- The OLCF team worked closely to provide timely access and throughput for full scale Gordon Bell runs.

Science Results

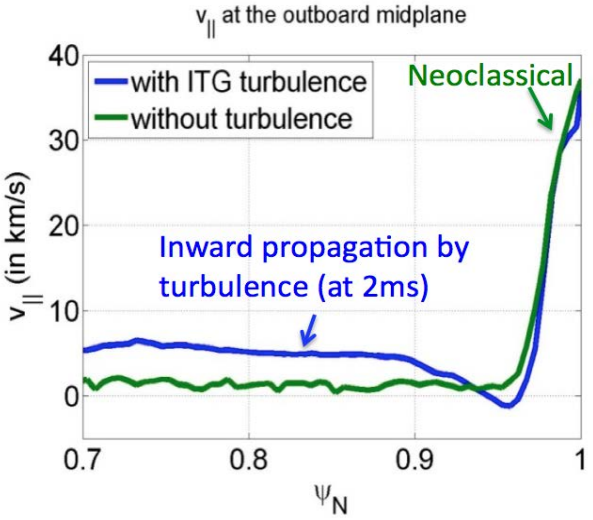
- Investigation of large-scale structure formation in the Universe with massive neutrinos and dynamical dark energy; focus on matter power spectrum predictions (submitted to Phys. Rev. D)
- Approximate neutrino treatment leads to negligible inaccuracy
- Large cosmological simulation with massive neutrinos, evolving 30 billion particles in 2.1Gpc cubed volume, analysis beyond power spectrum still ongoing
- High resolution simulation with latest Planck cosmology parameters currently being analyzed
- Supercomputing 2013 Gordon Bell finalist

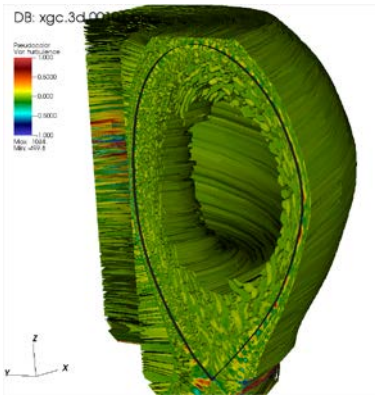
Generation of Intrinsic Toroidal Rotation in Tokamak Plasma to enable Stable Fusion Energy Production

C.S. Chang, Princeton
Allocation: 20,000,000

Science Objectives and Impact

- ITER plasma may need a toroidally rotating plasma for stable fusion energy production
- Application of an external torque is not efficient due to its large mass
- Intrinsic rotation source has been observed in the present day tokamaks, but not well-understood
- Generation of intrinsic rotation is a nonlinear multiscale problem in complex edge geometry
  - Turbulence, background evolution, neutral particles
- Large scale computing is necessary





Left: XGC1 identified an intrinsic edge rotation source and an inward momentum pinch phenomenon, similarly to experimental observations
Right: Nonlinear coherent turbulence transport momentum inward.

OLCF Contribution

- OLCF Liaison, Dr. E. D'Azevedo, helped porting of the fusion gyrokinetic code XGC1 to the heterogeneous Titan. As a result, XGC1 scales efficiently to the maximal Titan capability
- Dr. Pugmire of OLCF gave us a Vis support
- Ten-peta scale heterogeneous Titan enabled XGC1 to study the kinetic electron physics
  - Produced the gyrokinetic "blobby" turbulence

Science Results

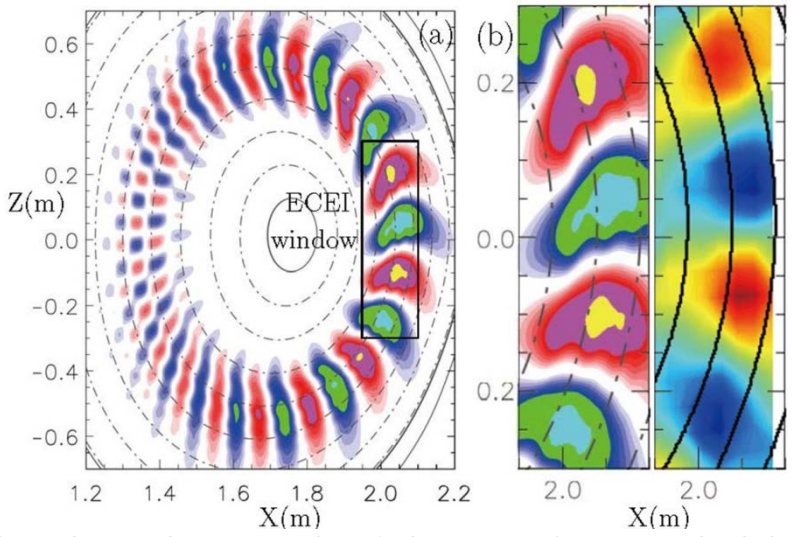
- Verified that a strong edge rotation source exist in H-mode pedestal, as observed in experiment.
- Verified that the rotation is pinched inward by turbulence, as observed in experiment.
- Produced the nonliear coherent edge turbulence structure, called "blobs" and "holes" from a gyrokinetic code for the first time.
- Identified that the rotation is carried inward by the "holes."
- Provides fundamental understanding of intrinsic rotation physics.

Predicting confinement properties of energetic particles in fusion reactor ITER

Zhihong Lin, UC Irvine
Award: 20,000,000 hours

Science Objectives and Impact

- Fusion can provide clean and renewable energy
- Energetic particles produced by fusion (α-particles) need to be confined in fusion reactor ITER
- Alfven eigenmodes excited by energetic particles cause loss of energetic particles
- This project develops simulation capability and physics understanding for predicting confinement properties of energetic particles in ITER



(a) Alfven eigenmode structure in a fusion reactor from GTC simulation. (b) Comparison of eigenmode structure from simulation (left) and from experiment (right) in ECEI measurement window (boxed region in panel a).

OLCF Contribution

- Porting GTC gyrokinetic particle code to titan computer and optimizing GTC for GPU
- Large scale GTC simulation to resolve kinetic effects in the magnetohydrodynamic instability (Alfven eigenmode)

Science Results

- Turbulent transport of energetic particles depends on the eigenmode structure and nonlinear dynamics of Alfven eigenmode
- GTC simulation finds a radial localization of the Alfven eigenmode
- GTC simulation finds a nonlinear oscillation of frequency and amplitude of the Alfven eigenmode

H. S. Zhang et al, Phys. Rev. Lett., 2012.
Z. X. Wang et al, Phys. Rev. Lett., 2013.

Computational Fluid Dynamics

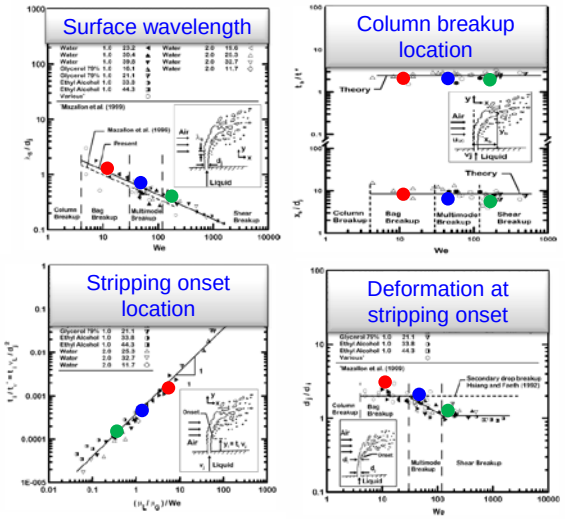
"High-fidelity Simulation of Spray Atomization"

OLCF
Oak Ridge Leadership Computing Facility

Xiaoye Li % M. Soteriou, UTRC
Award: 20,000,000 hours

Science Objectives and Impact

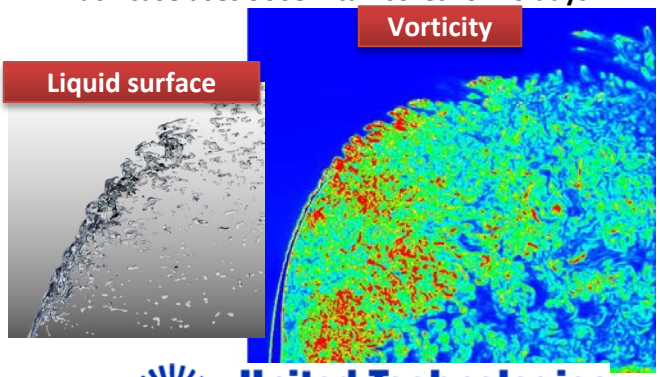
- Strategy: Employ High Performance Computing (HPC) simulation to study the atomization of liquid fuel by aerodynamic forces.
- Driver: Spray formation and evaporation play a key role in the performance, stability and emissions of aeroengine combustors. Limitations in experimental characterization point to first principles simulation as a viable analysis alternative. High simulation cost makes HPC a requirement.
- Objective: Perform high resolution simulation to validate a first principles method against experimental measurements - a first in the field.
- Impact: Establishes simulation-based *predictive* capability which can be used to enhance the design of fuel injectors and optimize combustor performance.



Prediction of atomization features compared with experimental data

Application Performance

- **3 validation cases of 500M grid each**
- **Each case uses 5008 Titan cores for 16 days**



United Technologies Research Center

Science Results

- For the first time, results from first-principle simulations are quantitatively validated against experimental data across a range of operating conditions.
- OLCF HPC enables high-resolution high-cost simulation and the demonstration of its ability to predict key, complex atomization phenomena seen experimentally.

Competitiveness Impact

Application of the simulation capability demonstrated in this project will lead to the development of next-generation fuel injection concepts which enable combustion systems with enhanced stability and efficiency, and reduced emissions.

OAK RIDGE National Laboratory

Liquid-Solid Interfaces in Electrocatalysis from First Principles

J. Greeley, Argonne National Laboratory

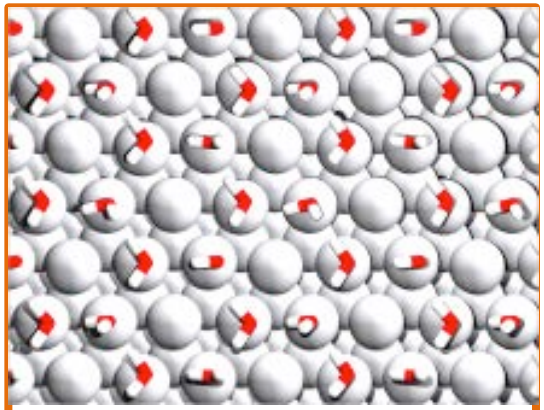
ALCC 2012-2013
20 M

Impact and Approach

- Investigate the structure and dynamics of chemical processes at the water/metal interfaces.
- Propose new catalysts with specific applications to environmental chemistry and other electrocatalytic problems (e.g. fuel cells and lithium ion batteries)
- DFT and force-field-based MD calculations.

Accomplishments

- Formation of water double-layer on Pt(111) surface demonstrated using DFT-based MD. Study simple adsorbates on Pt(111) surface. Implications for fuel cellls.
- Study nanoscale effects of lithium segregation in titania nanoparticles up to 10 nm in size. Study has implications for the use of titania as a next-generation anode in lithium ion batteries.



Water at a metal surface

ALCF Contributions

- DL-Poly compiled on Intrepid by Nichols A. Romero, catalyst.

Exploring the Nature of the Lightest Massive Particle in the Universe

Katrin Heitmann, Argonne National Laboratory

ALCC 2012-2013
10 M

Impact and Approach

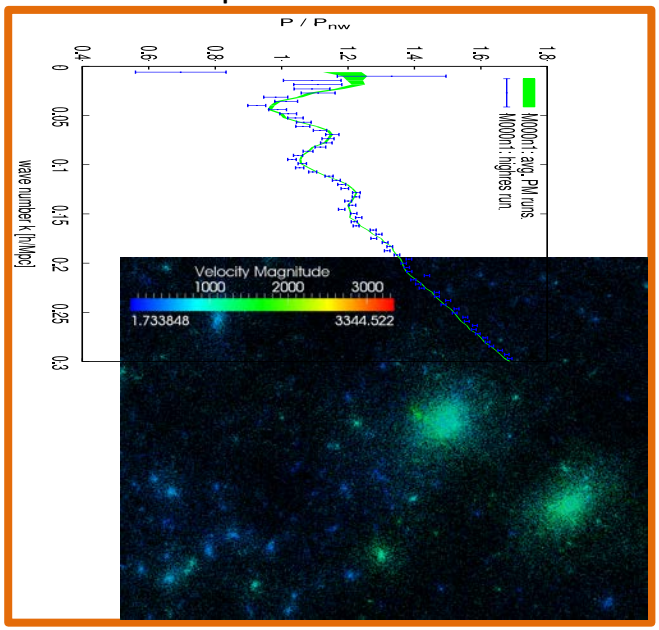
- Future cosmological measurements will be sensitive to the combined effects of dynamical dark energy and massive neutrinos
- Precision simulations including these effects are crucial to extract this information from observations
- Large mass difference between dark matter and neutrinos tracer particles poses numerical challenges for a two-species method
- Here: Develop approximate approach, show that it is accurate at the 1-2% level, investigate effects of neutrinos and dynamical dark energy on cosmological measurements

Accomplishments

- Investigation of large-scale structure formation in the Universe with massive neutrinos and dynamical dark energy (Upadhye et al. PRD)
- Approximate neutrino treatment leads to negligible inaccuracy
- Mass function investigation (Biswas et al. in prep.)
- Large scaling runs on Titan (SC13 Gordon Bell finalist)
- Suite of medium resolution simulations on Intrepid to investigate interplay between different parameters (Heitmann et al. in prep.)
- Titan simulation used to develop synthetic sky catalogs for large surveys

ALCF/OLCF Contributions

- OLCF: Support for fast turn-around of very large scaling runs for Gordon Bell submission
- ALCF: Implementation of neutrinos into HACC code by Adrian Pope and Hal Finkel



Power spectra from Intrepid and Titan runs (upper panel) and matter clustering in the Titan simulation (lower panel).

HPC Colony II
Terry Jones, Oak Ridge National Laboratory

ALCC 2012-2013
3 M

Impact and Approach

- Develop a new strategy to handle fault tolerance in the the recovery from communication failure.
- Using high-level information from the programming language, it is possible to avoid the use of "determinants", which are responsible of up to 20% overhead in the application.
- BG/P features unique multiple communication topologies, which is an important component in the load balancing testing, and allows to test the strategy at large scale.

Accomplishments

- New message-logging protocol with performance improvements of 50% to 75% were demonstrated at scale
- Better understanding of key meta-balancer tradeoffs between overhead and performance

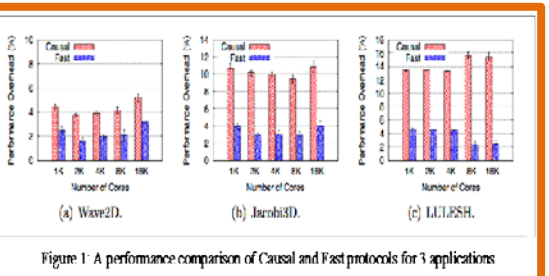


Figure 1: A performance comparison of Causal and Fast protocols for 3 applications

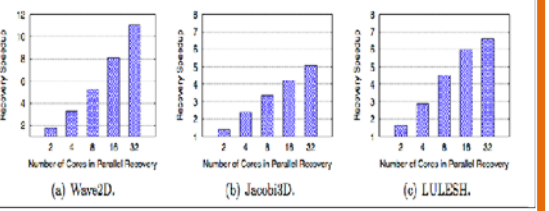


Figure 2: Recovery Speedup scalability by application.

ALCF Contributions

- Project was self sufficient and did not require ALCF contribution.

Petascale Thermal Hydraulic Simulations in Support of CESAR

Elia Merzari, Argonne National Laboratory

ALCC 2012-2013
30 M

Impact and Approach

- Numerical simulation is an intrinsic part of nuclear power plant R&D
- Center for Exascale Simulation for Advanced Reactors (CESAR) addresses computational software limitations for exascale hardware machines for the application of nuclear reactors
- Aim is to develop a coupled, next generation nuclear reactor core simulation tool capable of efficient computing at exascale
- This project uses today's petascale machines for benchmarking and analysis of thermal hydraulic reactor applications

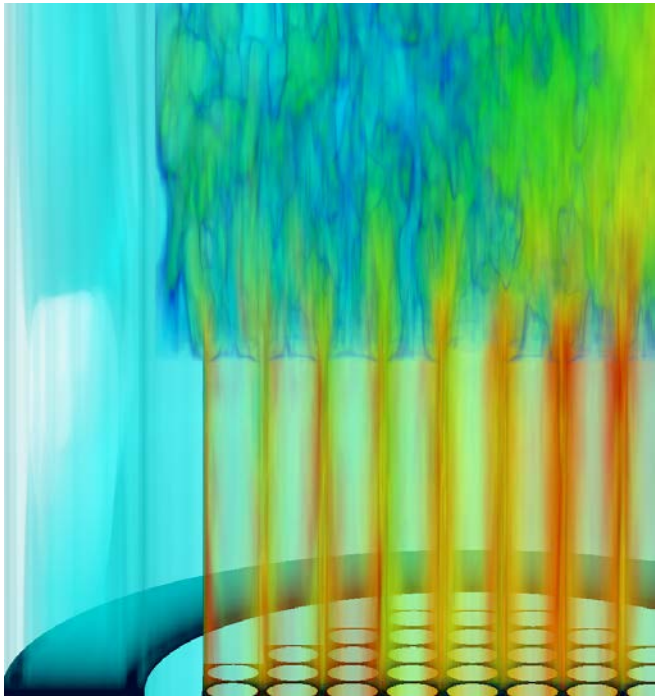
Accomplishments

- Developed and verified methodology to resolve wall shear stress in the flow of a nuclear reactor pin bundle for Large Eddy Simulations
- Simulated flow in 37-pin bundle using a very high-order polynomial/low-element count regime unusual for Nek5000. Scaling data collected as well as turbulence data.
- Simulated flow in Multi-Application Light Water Reactor test facility (MASLWR) to validate Nek5000 against experimental data

(Right) Flow in the core of the Multi-Application Light Water Reactor test facility (MASLWR) depicting axial velocity computed by Nek5000.

ALCF Contributions

- ALCF staff assisted with reservations critical to meet benchmarking deadlines.
- ALCF staff has worked closely with the Nek5000 team to port and optimize Nek5000 in past years.



Dynamics of Conformational Transition in Thermo-sensitive Polymers and Hydrogels

Subramanian Sankaranarayanan, Argonne National Laboratory

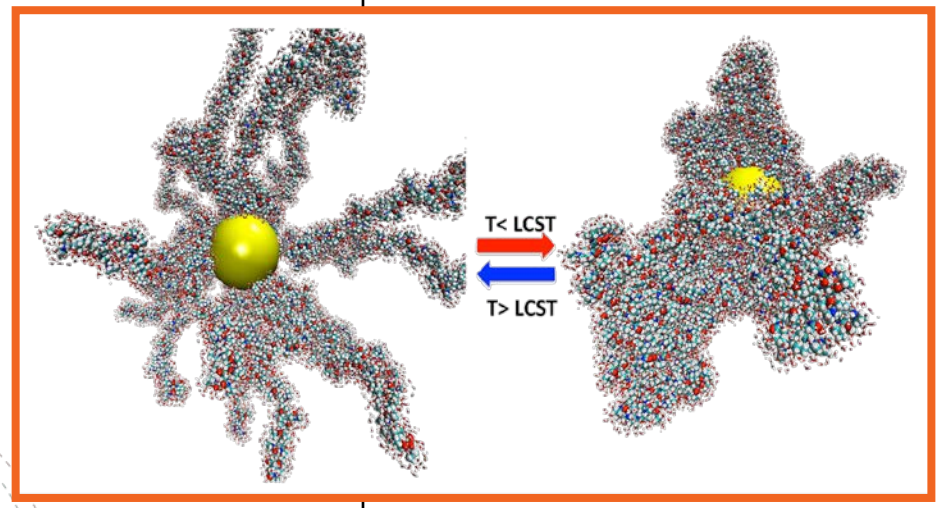
ALCC 2012-2013
50 M

Impact and Approach

- Fundamental understanding of stimuli response of smart polymers
- Identify role of solvation in inducing phase transition
- Design of controlled drug delivery systems

Accomplishments

- Identified the atomistic origin of coil-to-globule phase transition in thermosensitive polymers
- Ordering of water molecules is shown to play a critical role in dictating the polymer conformation
- Simulation results validated experimentally



ALCF Contributions

- ALCF recommended and built memory optimized version of NAMD for large scale computation.
- ALCF trained post-docs to use NAMD efficiently on Blue Gene/P (load balance parameters).
- ALCF fixed code that parsed input file and resolved a communication memory issue.

(Left) Simulations of temperature induced conformational change of polymer grafted gold nano-particle. 'LCST' or 'lower critical solution temperature' is the critical temperature for the conformational change.

Wall Modeling and Primary Atomization for Predictive Large-Eddy Simulation

Parviz Moin, Stanford University

ALCC 2012-2013
150 M

Impact 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 and vehicles.

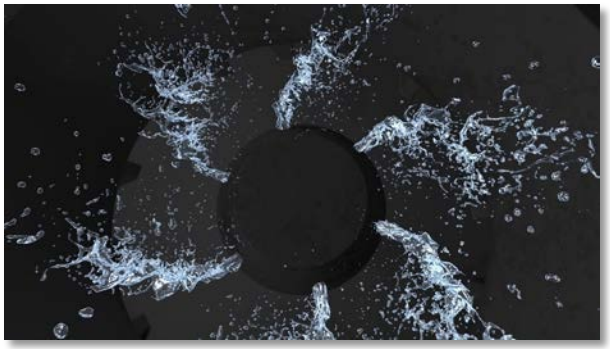
Accomplishments

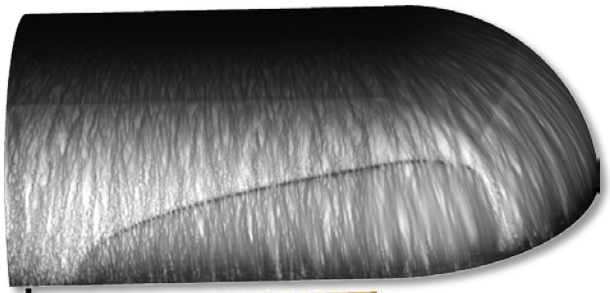
- LES models reproduce flight & ground test experiments for HIFiRE scramjet engine; unprecedented numerical database and validation.
- Novel wall-model tested on side-view mirror, validated against Honda experiments.
- Unstructured, exactly mass conserving VoF/Lagrangian scheme applied to full fuel injector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

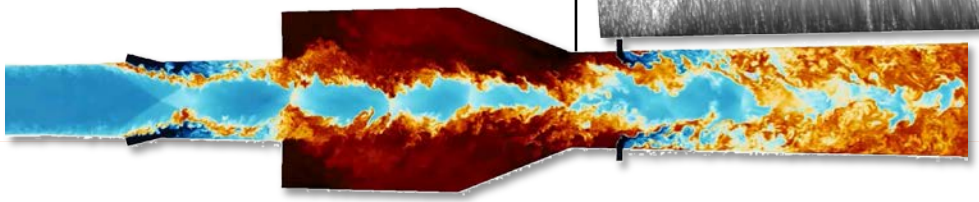
(Center) HIFire Scramjet Engine (Right, Top) Entire Swirling Fuel Injector (Right, Bottom) Automotive Side-View Mirror

ALCF Contributions

- Ramesh Balakrishnan and Vitali Morozov were instrumental in optimizing CharLES^{x} on Mira.







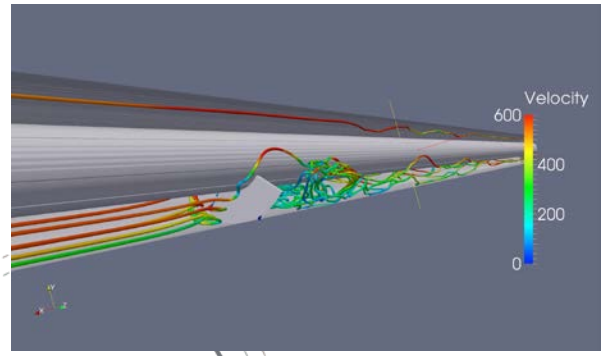
U.S.-Russia Collaboration on Verification and Validation in Thermal Hydraulics: Nek5000 and Conv3D Simulation of "SIBERIA" Experiment

Aleksandr Obabko, Argonne National Laboratory

ALCC 2012-2013
30 M

Impact and Approach

- SIBERIA experiment (Novosibirsk, Russia) has unique capability to provide high-precision, time-dependent measurements of near-wall flow for thermal hydraulics code validation exercises.
- Attractive experiment for international validation collaboration
- Cross verification/validation of Russian and U.S. codes



Accomplishments

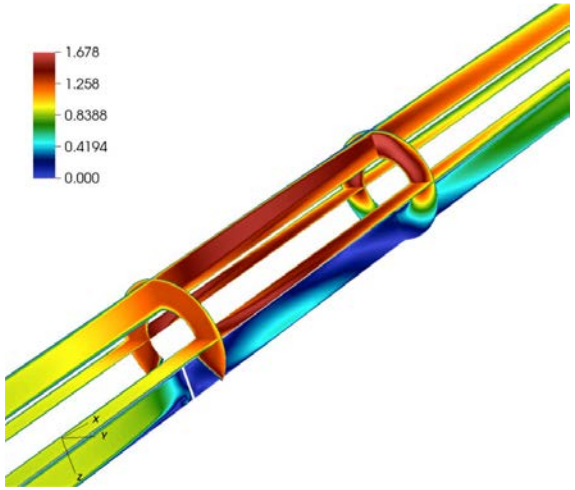
- Both Russian Conv3D team and U.S. Nek5000 team simulated flow in pin blockage geometry at moderate Reynolds number using Large Eddy Simulation (LES).
- Simulation results were analyzed and feedback was given to SIBERIA experiment team to agree upon measurement locations for validation this upcoming year.

(Left) Pathlines colored according to velocity experiment in Conv3D LES.

(Right) Velocity magnitude computed by Nek5000 LES.

ALCF Contributions

- Scott Parker and Joe Insley assisted with optimization of Nek5000 and visualization of data.
- Other ALCF personnel including ALCF management and support team helped establish and assist this collaborative effort between the U.S. and Russia.



Ab Initio Hyper-Nuclear Physics

Kostas Orginos, College of William and Mary

ALCC 2012-2013
20 M

Impact and Approach

- Study the spectrum of light nuclei and hypernuclei directly from the fundamental theory of strong interactions, QCD.
- Impact worldwide hypernuclear experimental program, as well as nuclear astrophysics, by refining our understanding of stellar evolution and core collapse.
- Calculations using Lattice Quantum Chromodynamics.

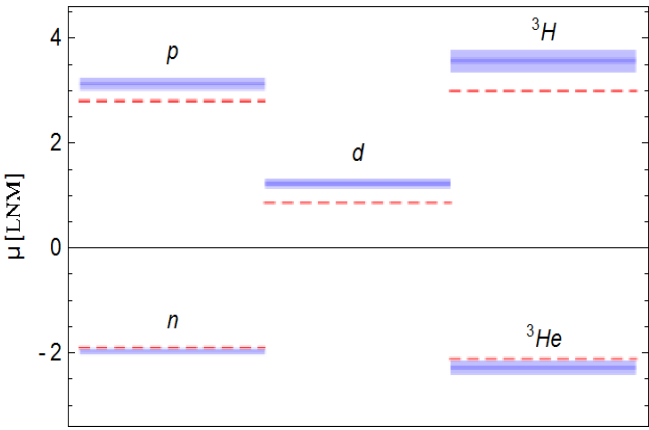
Accomplishments

- Produced an ensemble of 1500 gauge configurations to be used in future calculations of correlation functions.

(Right) The magnetic moments of the proton, neutron, deuteron, ^{3}He and triton. The lattice QCD results at a pion mass of about 806 MeV, are shown as the solid bands. The inner bands corresponds to the statistical uncertainties, while the outer bands correspond to the combined statistical and systematic uncertainties. The red dashed lines show the experimentally measured values at the physical quark masses.

ALCF Contributions

- ALCF Catalyst, James Osborn, helped diagnose and correct an issue with installing their I/O library.



Validation Work for Heterogeneous Reactor Calculations

Micheal A. Smith, Argonne National Laboratory

ALCC 2012-2013
30 M

Impact and Approach

- Goal is to simulate nuclear reactors in greater spatial detail
- Spatially detailed "heterogeneous" approach previously untenable due to large resource requirements and lack of available codes
- DOE NEAMS PROTEUS code uses novel algorithms to leverage leadership computing resources
- Can solve problems in unprecedented detail on DOE supercomputers
- Early studies on computational requirements now being performed in preparation for future validation and multi-physics coupling work

Accomplishments

- Due to funding shifts, work shifted from validation to demonstration problems
- Demonstrated partially heterogeneous full core "pseudo" transient where reactor core undergoes prescribed inlet temperature perturbation
- Initiated convergence study of asymmetrical CANDU-like heterogeneous reactor problem
- Assessed computational effort required for continuous FEM codes on heterogeneous thermal reactor problems

(Right) Power profile of pseudo transient at initial condition showing heterogeneous assembly

ALCF Contributions

- P. Rich assisted with setting up sub-block jobs.
- R. Loy assisted with use of debuggers.
- E. Wolters and V. Viswanath met to discuss improvements to parallel I/O strategy.