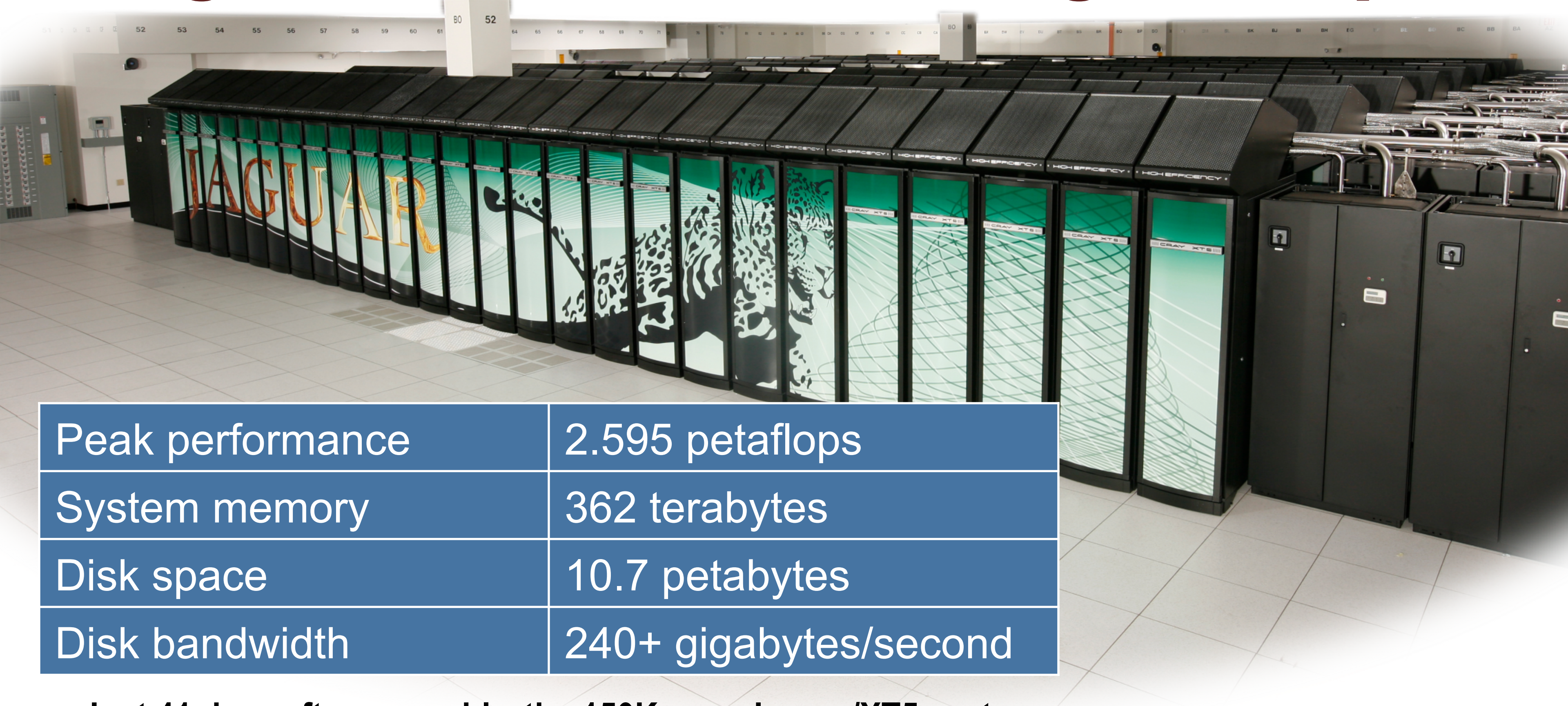
OLCF Science Overview

Presented by

Bronson Messer

Astrophysicist, OLCF

Jaguar: World's most powerful computer Designed for science from the ground up



Peak performance	2.595 petaflops
System memory	362 terabytes
Disk space	10.7 petabytes
Disk bandwidth	240+ gigabytes/second

- **Just 41 days after assembly, the 150K-core Jaguar/XT5 system:**
  - **Had two real applications running over 1 PF**
    - **DCA++ (1.35 PF): high temperature superconductivity**
    - **LSMS-WL (1.05 PF): thermodynamics of magnetic nanoparticles**

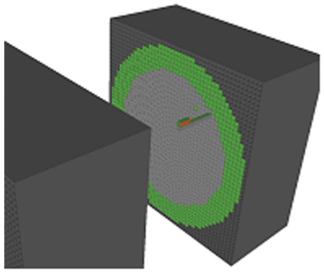
Dinesh Kaushik
ANL

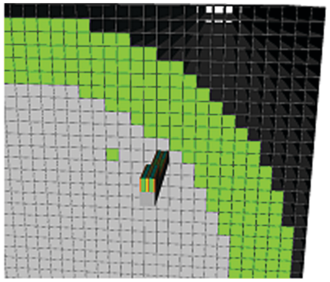
Nuclear Engineering

Scalable Simulation of Neutron Transport in Fast Reactor Cores

Science Objectives and Impact

- Perform detailed, high-resolution simulations of neutron transport in fast reactor cores using the UNIC code, being developed as part of the DOE Nuclear Energy Advanced Modeling and Simulation Program.
- To model the complex geometry of a reactor core, billions of spatial elements, hundreds of neutron directions ("angles"), and thousands of neutron energy groups are necessary, which leads to problem sizes with petascale degrees of freedom. Such calculations are not possible without large- scale parallel platforms such as Jaguar. Through these high-fidelity simulations, the team aspires to
  - (1) free reactor designers to explore innovative design concepts with minimal need for new physical "calibration" experiments and
  - (2) reduce uncertainties for existing designs to enable more economically efficient design/operation.
- Fast reactors—which do not use a moderator to slow the neutrons that split fissile nuclei— show promise as both a source of electrical power and one producing minimal nuclear waste.





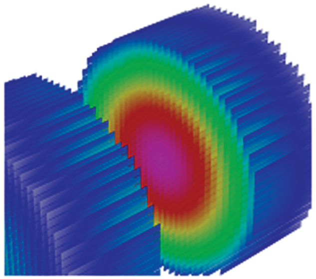


Image Caption

Two pictures (left and center) of ZPR 6/6A geometry and uranium-235 plate power distribution (with separated matrix halves). The gray indicates the matrix tube and drawer fronts that are loaded into each tube position. The solid green squares are 2 in. depleted uranium metal blocks directly loaded into the tubes surrounding the main core and acting as a neutron blanket. The plot at the right shows the enriched uranium plate power with the matrix halves separated. Images courtesy of Dinesh Kaushik, ANL.

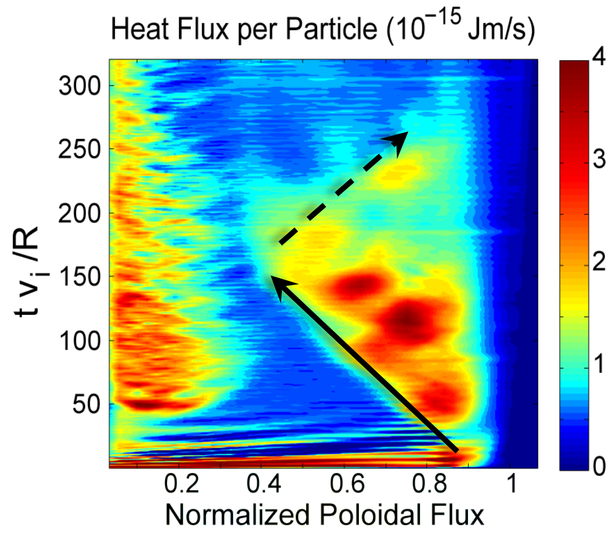
C.S. Chang
New York Univ.

Fusion energy science

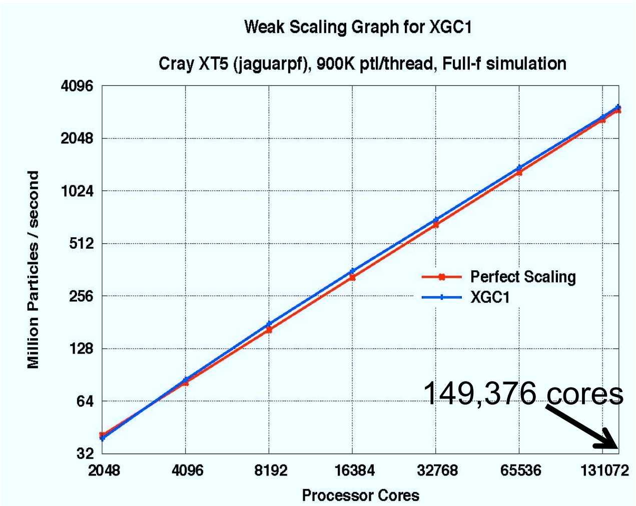
Core-edge nonlocal profile formation of tokamak plasma

Science Objectives and Impact

- **Obtain first-principles understanding on the fusion efficiency of tokamak reactor plasma using extreme scale HPC**
- **Edge conditioning, which may be the only mean to control the reactor plasma, has been ubiquitously observed to improve the core plasma profile dramatically in experiments.**
- **Multiscale nonlocal core-edge simulation of the combined ion-temperature-driven turbulence dynamics and the background ion-temperature profile evolution in realistic DIII-D device geometry in a day.**
- **Open up a door to practical first-principles predictive simulation capability for ITER and DEMOs**



XGC1 Performance



Science Results

- **World's only whole volume turbulence simulation in realistic tokamak geometry.**
- **Core turbulence is sum of the incoming intensity from edge and the ambient local fluctuations, self-organizing the temperature gradient in turbulence propagation time scale (similar to experiments).**

Image Caption

Shown above is the turbulent heat flux in time and radius (normalized flux). Turbulence propagates from edge to core (solid arrow), induces outward heat flux (dashes arrow), and leads to an eventual new self-organized nonlocal state.

Lin-Wang Wang
LBL

Solar energy science

Harnessing the power of our star

Science Objectives and Impact

- Simulate solar panel materials at the atomic level, where both inefficiencies and possible improvements begin
- Investigate ways to increase theoretical photovoltaic (PV) cell efficiency.
- Push photovoltaic cell technology forward, accelerating the understanding of new PV nanocells.
- LS3DF algorithm scales linearly and in parallel, making it an ideal software tool for jaguar.

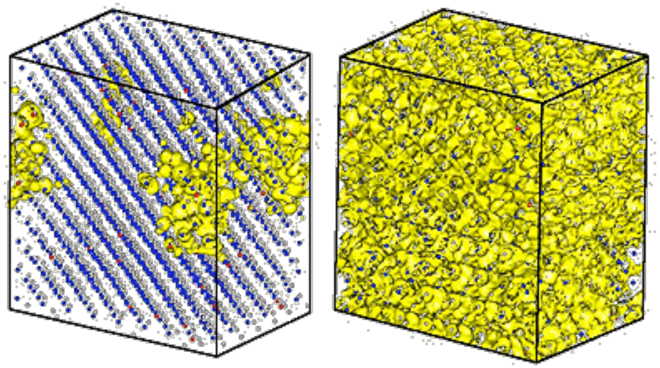
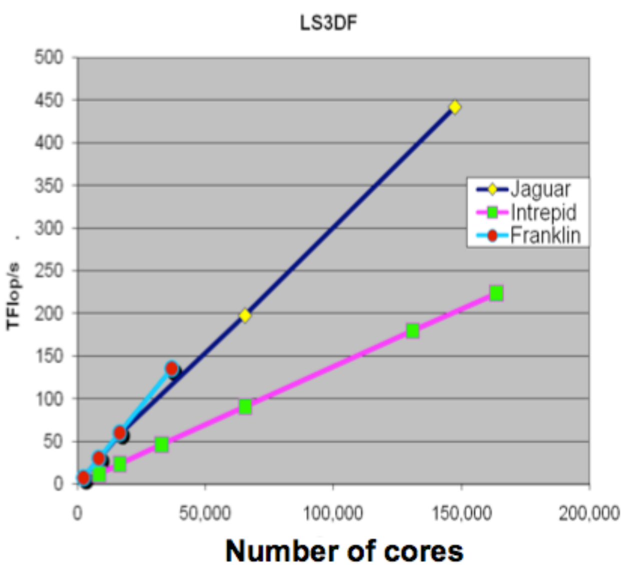


Image Caption
Intermediate electron states in zinc tellurium band gap introduced by the introduction of oxygen into the alloy. The electrons shown in the right image are in the conducting band, and can conduct electricity.

LS3DF Performance



Science Results

- Introduction of oxygen into zinc-tellurium alloy produces a new band within the original band gap.
- The resultant additional electron states are very localized, leading to superior conduction properties.
- Localized new state provides a “stairstep” inside the band gap of the material while preventing electron relaxation into phonons.
- New intermediate state can increase the theoretical effiency of PVC from 30% to 60%

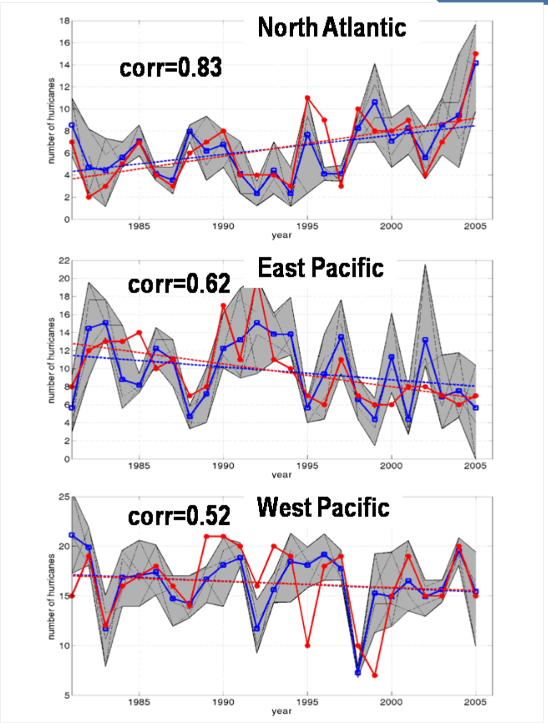
Venkatramani
Balaji
NOAA/GFDL

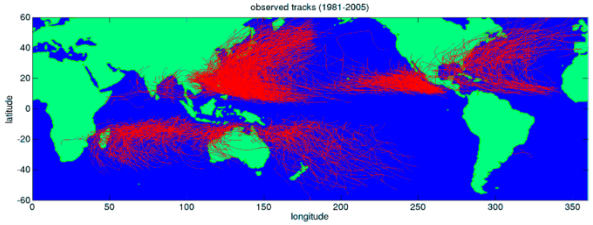
Climate Science

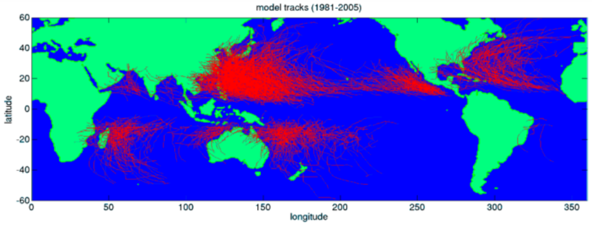
Exploring the limits of climate prediction

Science Objectives and Impact

- A team led by GFDL climate scientist Venkatramani Balaji is using Jaguar to simulate and assess both natural and anthropogenic causes of climate change at exceptional resolutions.
- Current resolutions of IPCC–class models are mostly in the 100-kilometer range, but Balaji's research team seeks to create models in the 25- to 50-kilometer range, allowing regional climate prediction.
- Two scientific themes emphasized in this Coupled High-Resolution Modeling of the Earth System (CHiMES) project are decadal predictability of the Earth System and correlation of tropical cyclone frequencies and intensities with climate change.
- The cutting edge of climate research and policy questions is now moving to the issue of understanding and predicting climate variability and change on regional scales. Such regional scales are the ones of most direct relevance to society and decision makers.







HiRAM captures bothe the inter-annual variability and decadal trend over the North Atlantic, the East and West Pacific.

Red: observations

Blue: HiRAM ensemble mean

Shading: model spread

Image Captions

Simulation of global hurricane climatology and response to global warming in a new global High Resolution Atmospheric Model (HiRAM) at 50-kilometer resolution. Images courtesy: Ming Zhao, Isaac Held, Shian-Jian Lin, Gabe Vecchi, NOAA/Geophysical Fluid Dynamics Laboratory

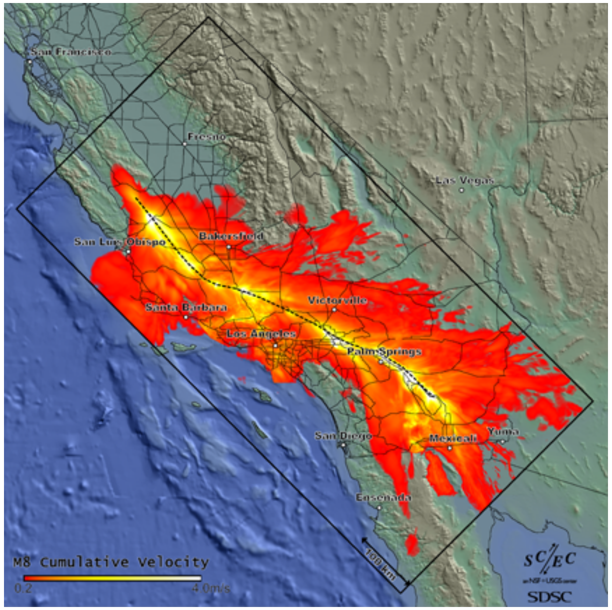
Thomas Jordan
USC

Earth science

Deterministic Simulations of Large Regional Earthquakes

Science Objectives and Impact

- Prediction of ground velocity and seismic wave propagation is essential to understand the impact of large earthquakes.
- Earthquake ground motion simulation useful for
  - Emergency management agencies evaluating "worst case" earthquake scenarios for California
  - Building engineers evaluating tall building response to possible future earthquakes
  - Seismic network operators evaluating whether their current station distribution provides adequate monitoring for large earthquakes
  - Seismic hazard modeling groups evaluating how 3D ground motion simulations capture ground motions caused by earthquake directivity and basin amplifications.



M8 simulation specs

435 billion 40-cubic-meter cells

frequency of the seismic waves followed up to 2 Hz (each doubling of frequency requires 16x increase in computing power)

Science Results

- SCEC project simulates a 6-minute earthquake half again as powerful as the temblor that destroyed San Francisco in 1906 -- or 30 times as powerful as the quake that devastated Haiti in January.
- Ensemble of realizations provide statisitcal measureof uncertainty in ground motion predictions – immediately useful to engineers building for earthquake resilience

Image Caption
Cumulative ground velocity from simulated magnitude 8.0 earthquake in Southern California.

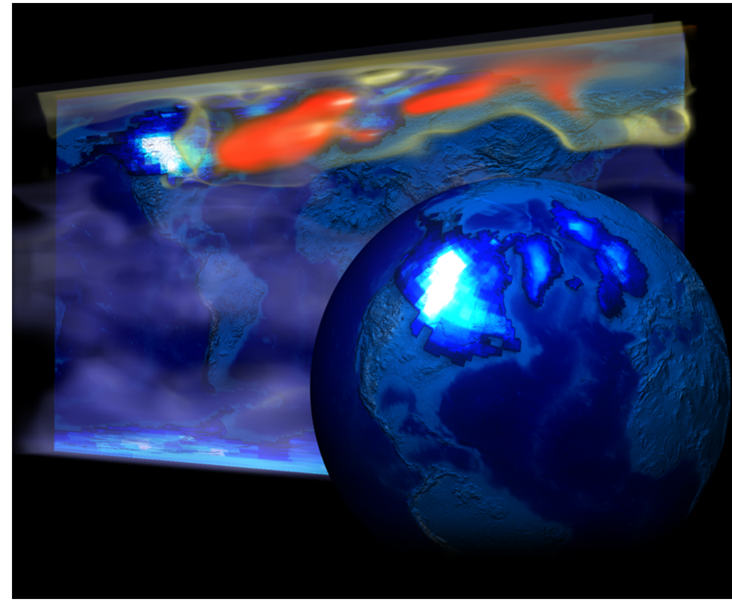
Zhengyu Liu
Univ. Wisconsin

Climate science

Validating the tools for studying climate change

Science Objectives and Impact

- The ability to use climate models to predict future events relies on validating those models with data from the past
- Abrupt changes in climate provide an especially inviting target for model validation.
- Petascale computing enables continuous (over millennia) simulations to capture transient low-probability events.
- CCSM framework provides necessary physical models and code base to perform such validation experiments.



IPCC
INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE

The data from OLCF simulations may soon find their way into IPCC's data repository and reports as the community assesses our understanding of, and ability to realistically simulate, Earth's climate system.

Science Results

- First continuous simulation of climate change spanning from 21,000 to 14,000 years ago, capturing the Bølling-Allerød warming – the most recent period of natural warming.
- Understanding natural abrupt climate change can provide insight into ocean circulation changes possible from anthropogenic warming now.

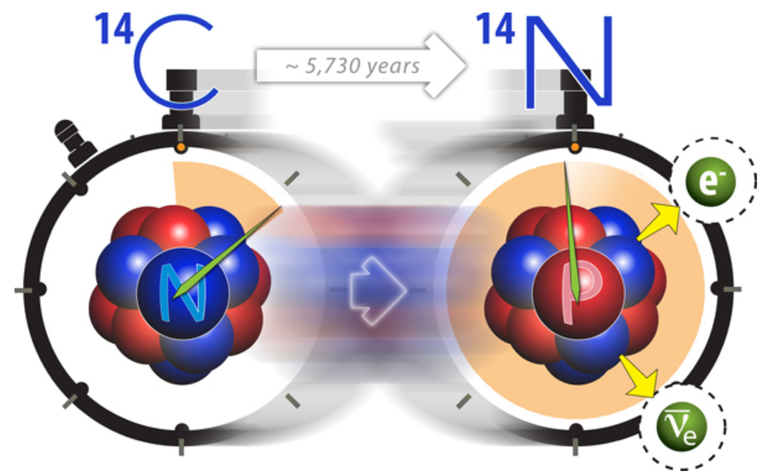
Image Caption
Simulations showing deglaciation during the Bølling-Allerød, Earth's most recent period of natural global warming.

David Dean
ORNL

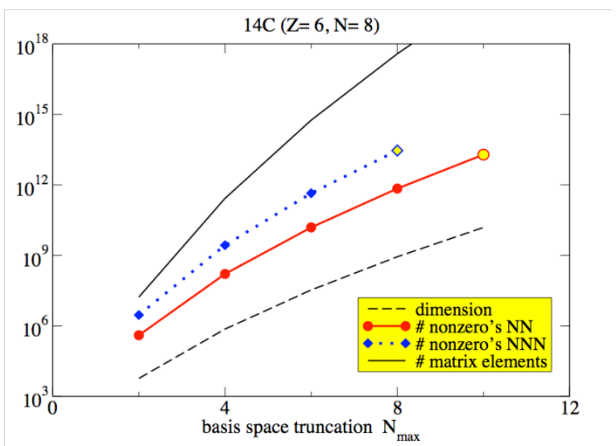
Nuclear physics
Understanding nature's premier clock

Science Objectives and Impact

- Carbon-14 (^{14}C) dating has proven to be the most reliable method to date a variety of relics from the past because of its anomalously long half-life.
- Nuclear shell model calculations that use models of lighter elements do a poor job of reproducing the half-life of ^{14}C.
- More sophisticated potentials and solution methods can now be brought to bear on the problem.
- Complete understanding of ^{14}C structure underscores confidence in the use of ^{14}C to date a multitude of artifacts from human prehistory and before.



MFDn memory requirements



Introduction of three-body potentials requires more than 300TB of memory

Science Results

- *Ab initio* methods, stemming directly from the strong interactions between constituent quarks, and the introduction of three-body and above interaction potentials begin to bridge the gap between nuclear structure and QCD.
- Same techniques can be applied to a variety of other nuclei as well, increasing our understanding of the basic constituents of nature.

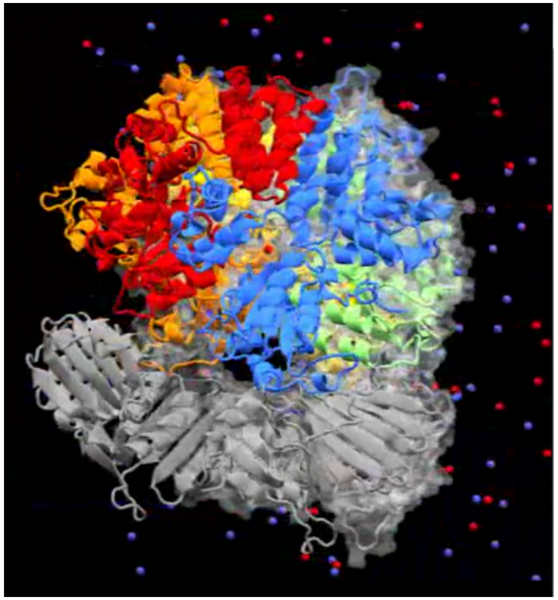
Ivaylo Ivanov
Ga. State Univ.

Bioscience

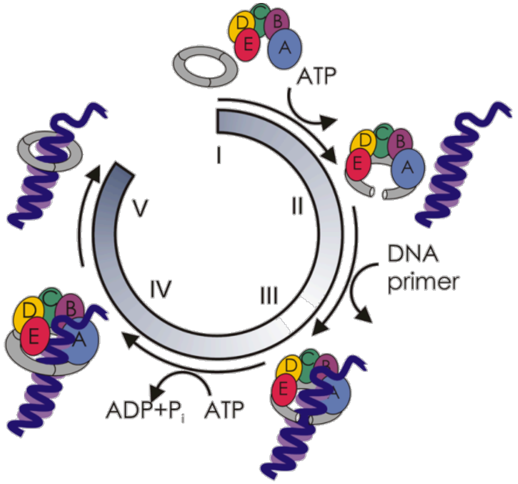
Molecular Machines Replicate and Repair DNA

Science Objectives and Impact

- A research team recently used Jaguar to elucidate the mechanism by which accessory proteins called sliding clamps are loaded onto DNA strands and coordinate enzymes that enable gene repair or replication.
- Simulating just a few pieces of the replisome - the molecular machinery responsible for the faithful duplication of genetic material during cell division – requires modeling more than 300,000 atoms.
- An improved understanding of the replisome may make it possible to exploit differences among organisms as diverse as viruses, bacteria, plants, and animals for drug design.



Clamp Loading Cycle



Science Results

- Simulations reveal a ring-shaped protein known as a proliferating cell nuclear antigen, or “sliding clamp” to biologists, plays a pivotal role in replication.
- Research has direct bearing on understanding the molecular basis of genetic integrity and the loss of this integrity in cancer and degenerative diseases

Image Caption

Supercomputers at the OLCF illuminate the workings of the molecular machinery that opens and loads sliding clamps onto DNA. Sliding clamps play vital roles in both DNA replication and repair. Here the clamp loader (with its subunits shown in blue, green, yellow, orange, and red) is depicted in complex with a ring-open sliding clamp (shown in gray) and counterions (spheres). *Image courtesy Ivaylo Ivanov and Mike Matheson*

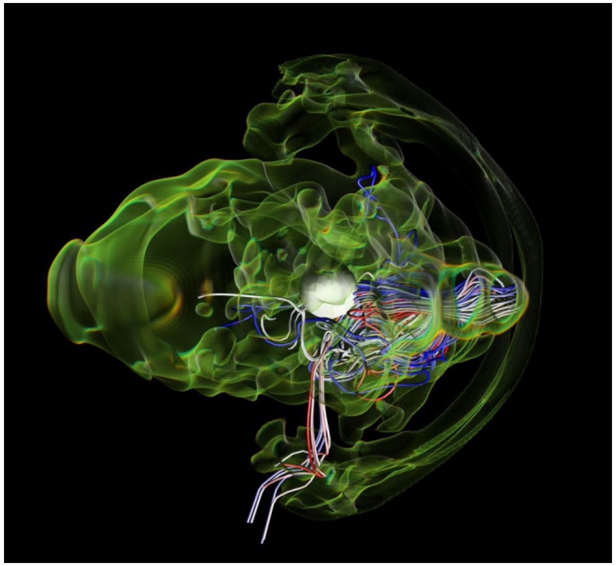
Anthony Mezzacappa, ORNL

Astrophysics

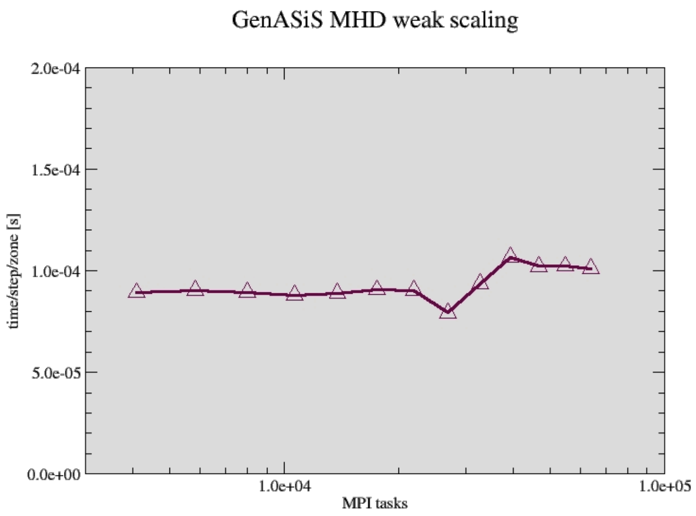
The role of magnetic fields in the birth of pulsars

Science Objectives and Impact

- Stationary accretion shock instability (SASI), a computational discovery from earlier INCITE work, is a potential source of spin for pulsars
- However, pulsars also have strong magnetic fields that power their synchrotron emission, making them cosmic lighthouses
- Endeve, et al. ApJ 713 (2010) 1219



GenASiS Performance



Science Results

- Large (~100,000 processors) MHD simulations performed with GenASiS show that rapid field amplification does occur, driven by the turbulence caused by the SASI
- SASI induced rotation and magnetic fields can produce pulsars even from non-rotating progenitor stars
- Confirmed that the general dynamic features of the SASI remained unchanged by magnetic fields

Image Caption
Magnetic field streamlines from a MHD simulation of the stationary accretion shock instability in core-collapse supernovae

Dario Alfe
UCL

Materials Science:

Computational Surface Science at High Accuracy with Quantum Monte Carlo

Science Objectives and Impact

- A team of researchers from University College London are using Jaguar to obtain a full-binding energy curve between water and graphene.
- Most natural surfaces are covered by a film of water— science could greatly benefit from a more precise explanation of such systems simply because they occur so often in the natural world.
- The team received 2 million hours on Jaguar to calculate a water molecule's adsorption energy and geometry on a sheet of graphene. Adsorption is the accumulation of atoms or molecules on the surface of a material.
- By calculating the adsorption energy and geometry in 30 individual steps as the molecule moves closer to the surface, the team made history with their results.

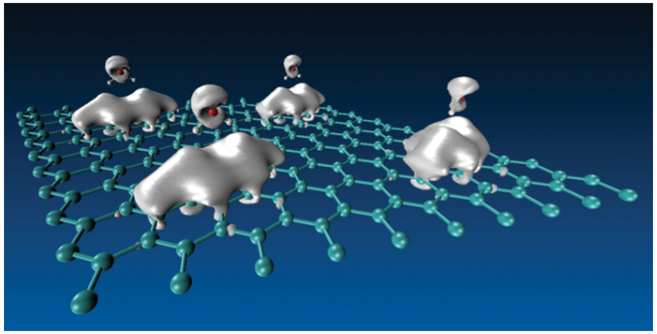
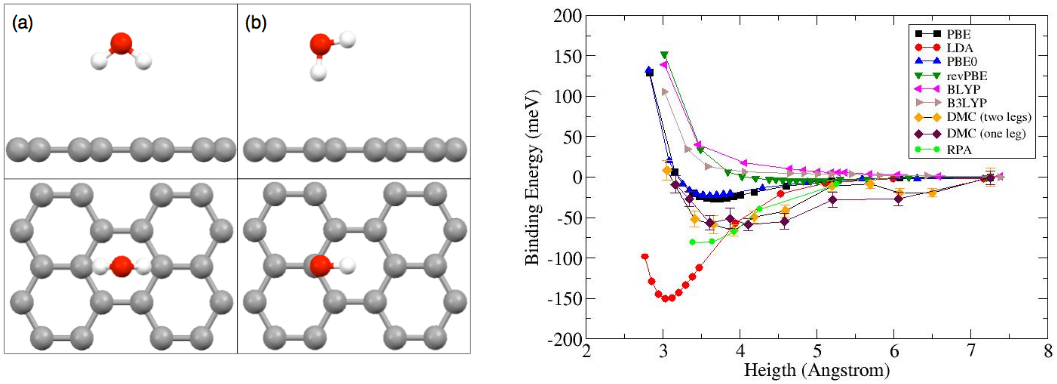


Image Caption
The image above shows how electrons rearrange when four water molecules bond to a sheet of graphene. Image courtesy Dario Alfe, University College London

Application Performance



DMC results now compared with standard quantum mechanics calculations based on density functional theory, with varuious exchange-correlation functionals. The spread of the latter results, some of which even predict no binding at all, shows the need for a more accurate technique like DMC to obtain reliable results for this system.

Science Results

- Completion of the calculation of the full binding energy curve between a water molecule and an graphene layer.
- Three million hours. Highly accurate quantum Monte Carlo simulations based on the Diffusion Monte Carlo (DMC) method. Simulation results: binding energies of 70 +- 20 meV (see next two slides)

Mike Henderson
BMI Corp.

Computational Fluid Dynamics

"Smart Truck Optimization"

Science Objectives and Impact

- Apply advanced computational techniques from aerospace industry to substantially improve fuel efficiency of Class 8 Long Haul Trucks
- New California Air Resources Board (CARB) requires 5% fuel efficiency increase on all Class 8 trucks; national drive to reduce emissions.
- Determine type and design of add-on parts to substantially reduce drag / increase aerodynamic efficiency
- If all 1.3 million long haul trucks operated with the drag of a passenger car, the US would annually:
  - ü Save 6.8 billion gallons of diesel
  - ü Reduce 75 million tons CO_2
  - ü Save $19 billion in fuel costs

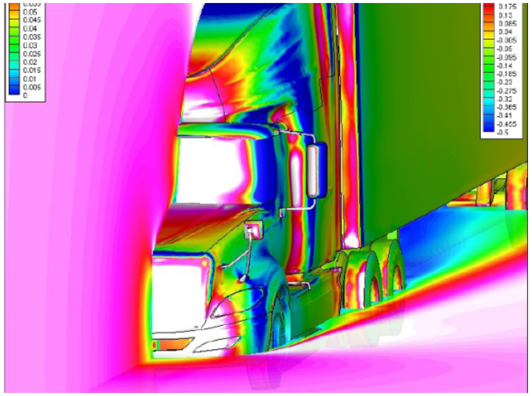
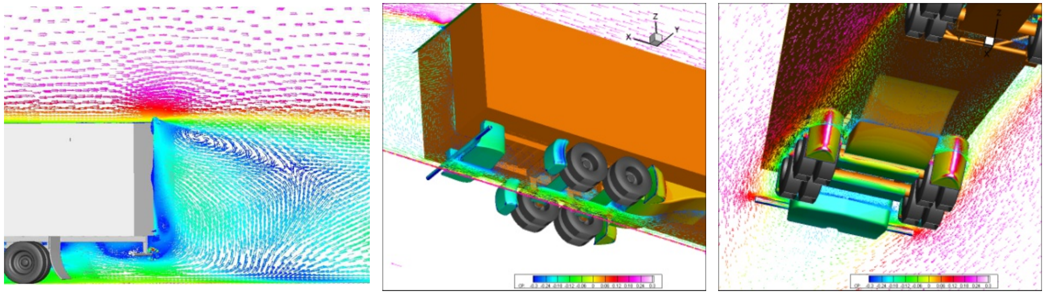


Image Caption
Pressure around SmartTruck design.



UT-6 Trailer UnderTray System

- CFD results using NASA'a FUN3D within 1% of physical test results
- Access to Jaguar reduced single run times from 15 hours to less than 2 hours
- Stage set to do full Navier Stokes based optimization of large trucks

Science Results

Unprecedented detail and accuracy of a Class 8 Tractor-Trailer aerodynamic simulation.

UT-6 Trailer UnderTray System reduces Tractor/ Trailer drag by 12%.

- Minimizes drag associated with trailer underside components
- Compresses and accelerates incoming air flow and injecting high energy air into trailer wake
- Pulls high energy, attached air flow from the top of the trailer down into trailer wake

Nanoscience / nanotechnology

M. Luisier, G. Klimeck, Purdue Univ.

Petascale simulations of nano-electronic devices

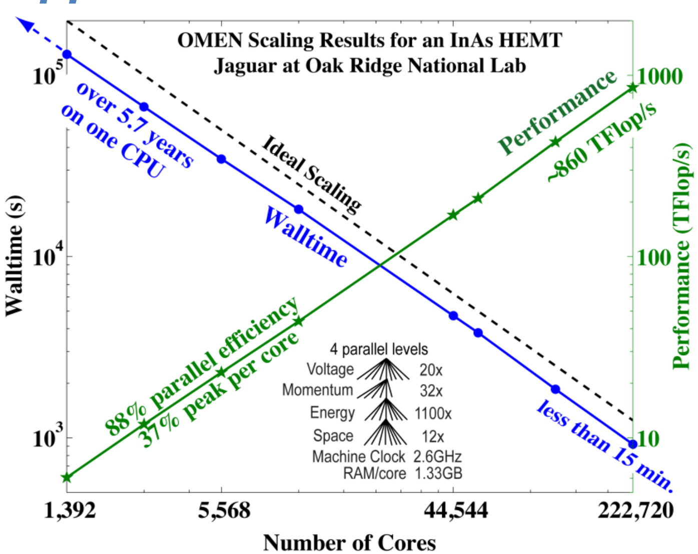
Science Objectives and Impact

- Model, understand, and design carrier flow in nano-scale semiconductor transistors. Represent structure one-atom-at-a-time consistent of tens of thousands of atoms and simulate fully quantum mechanically with non-equilibrium Green function formalism for transport
- Identify next generation nano-transistor architectures. Reduce power consumption and increase manufacturability.
- Move nano-science to nanotechnology through computing.
- Demonstrate full atomistic quantum transport simulations. Coherent transport in a few minutes, scattering transport hours at the peta-scale.

Science Results

- Coherent transport simulations in band-to-band tunneling devices with simulation times of less than an hour
  => rapidly explore design space
- Incoherent transport simulations coupling all energies through phonon-interactions. Production runs on 70,000 cores in 12 hours
  => first atomistic incoherent transport simulations
  => understanding source control

Application Performance



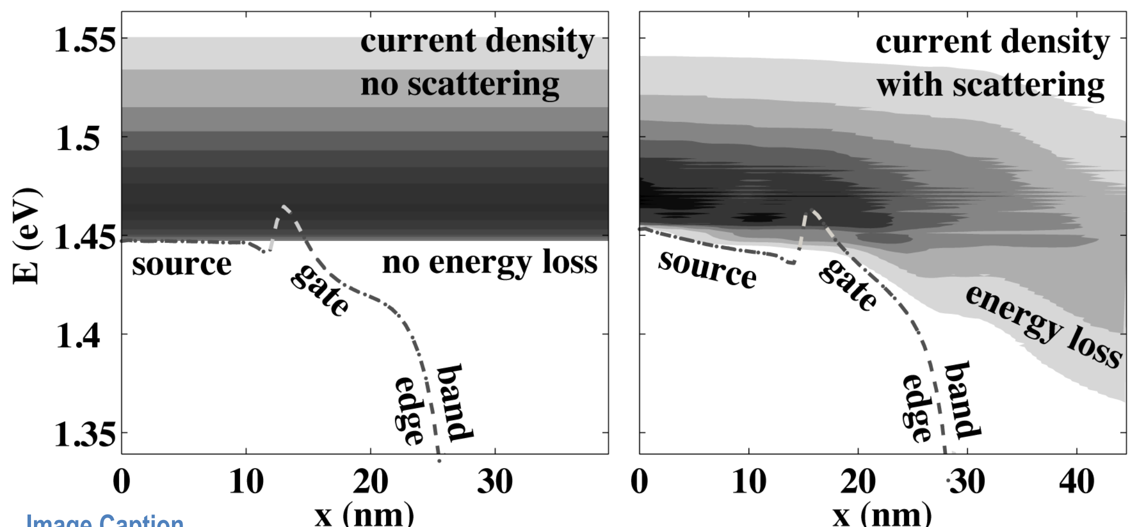


Image Caption

Energy-resolved current distribution in nano-scale transistor.

Left: coherent transport with out energy loss.

Right: with phonon scattering. Carriers lose energy and modify energy bands at source.

Contact

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