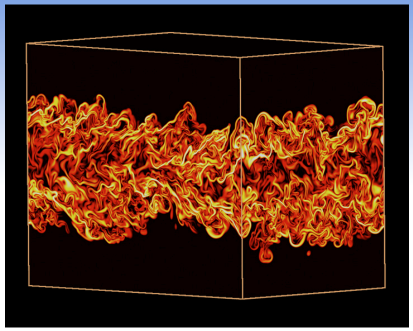
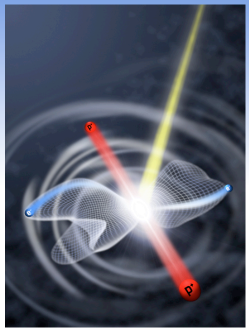
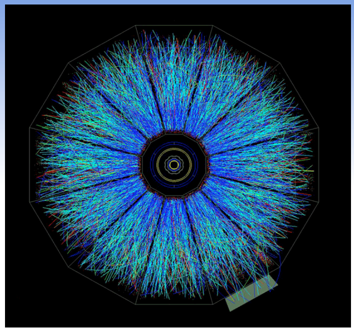
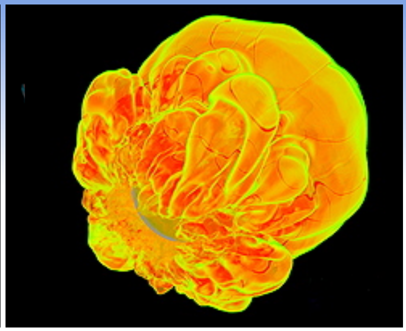






Selected NERSC Science Highlights 2009

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC

BERKELEY LAB

Material Science: Optical Data Storage

Objective: Explore ultrafast optical switching of nanoscale magnetic regions.

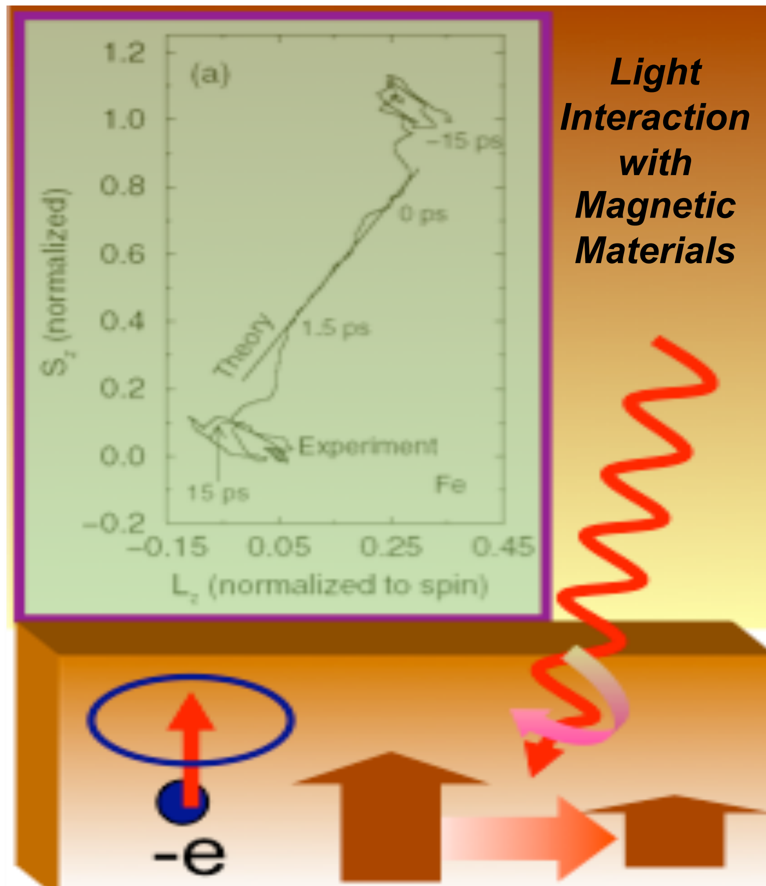
Implications: Potential for laser operated hard drives, 1000s of times faster than today's technology.

Accomplishments: First-principles, time- & spin-dependent DFT study using locally-designed code on laser-irradiated Ni.

- Discovered that light leverages the crystal structure to transfer spin of electrons to higher orbit.
- Study is the first to clearly demonstrate that this phenomenon is a relativistic effect connected with electron spin.
- Discovery matches experiment and can guide synthesis of new materials.

NERSC:
- 1.5 M hours in 2009; typically using 2,800 cores.

PI: G. Zhang (Indiana St)



J. Appl. Phys. (2008)

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Chemistry: Nanoparticle Catalysis

Objective: **Study small metal clusters supported on nanoparticles to understand heterogeneous catalysis; help design improved catalysts.**

Implications: **Better hydrodesulphurization in power plants; possible conversion and use of non-conventional fuels, e.g., MeOH.**

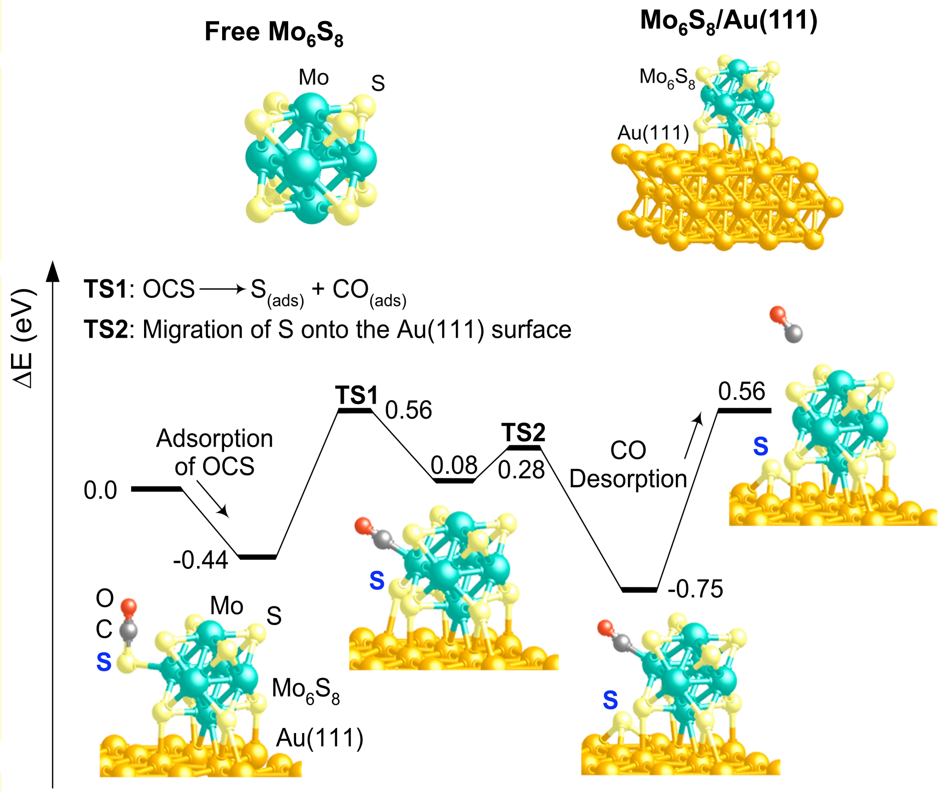
Accomplishments: **DFT calculations and state-of-the-art cluster beam studies provide insight into the reaction mechanism of catalytic activity of molybdenum-sulfur clusters on gold surfaces.**

- **Help identify intermediates along the catalytic reaction pathway.**

NERSC:

- **700k hours thus far 2009**
- **Uses ORNL / NERSC version of VASP**

PI: P. Liu (BNL)



Potential energy profile for the interaction of CarbonylSulfide (OCS) on Mo_6S_8 / Au(111)

J. Am. Chem Soc., *submitted*

Nuclear Physics: Lattice QCD

Objective: **Understand strong interactions that bind quarks and gluons together.**

Implications: **Explain new phases of matter that might form in heavy-ion collisions (in LHC, for example).**

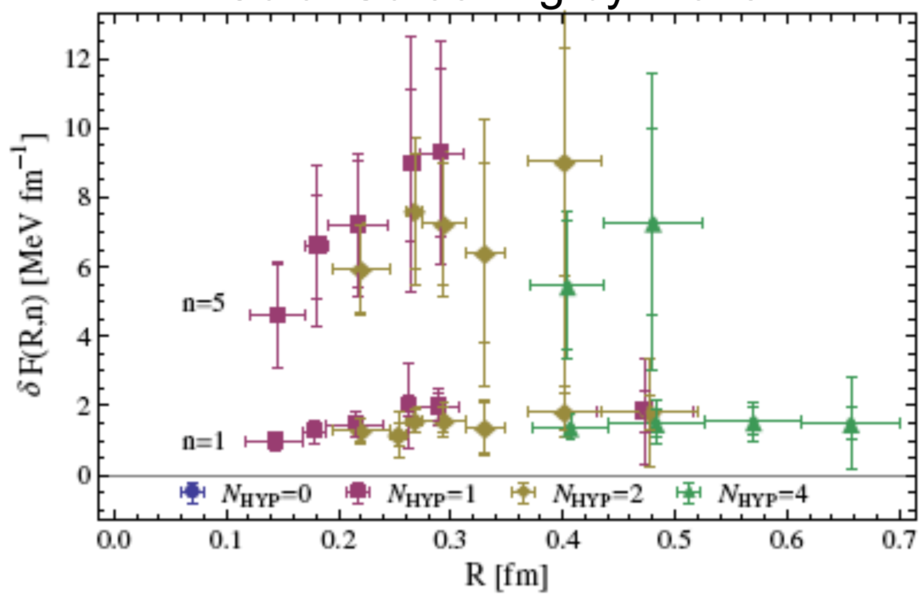
Accomplishments: **Cited by DOE in 2010 Congressional Budget Request as one of 3 major accomplishments in Theoretical Nuclear Physics in 2008/9.**

- **First ever QCD calculations of:**
  - **Three-body force between hadrons.**
  - **Screening of color forces between quarks by a background of hadrons.**
  - **a three-baryon system.**

NERSC:
- **QDP++/Chroma on Franklin; 10M+ hours**
- **Mostly 4k cores per job**

PIs: M. Savage (U. Wash.), W. Detmold (JLab, College of W&M)

Color Screening by Pions



Contribution to the radial quark-antiquark force at two pion densities. The attractive force is found to be slightly reduced by the presence of the pion gas. This is a first step toward a more systematic exploration of hadronic effects with lattice QCD.
("Pion" is short for pi meson.)

Phys Rev Lett, (2009)

Materials Science: Nanostructures

Objective: **design, simulate and help realize nanoscale molecular transport systems.**

Implications: **Possible use in drug delivery, advanced sieves, desalination.**

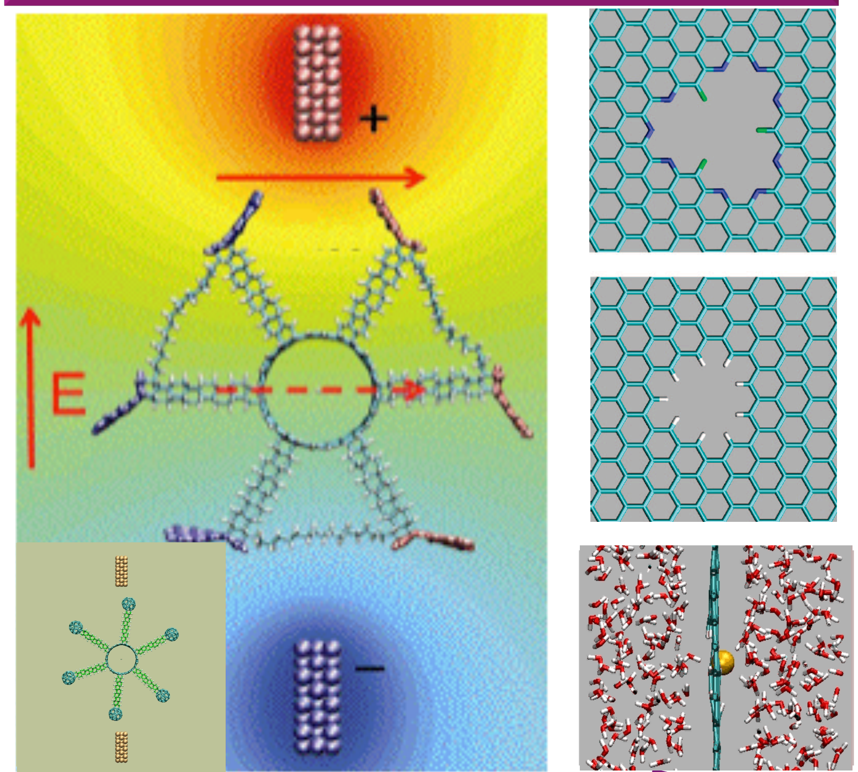
Accomplishments: **Simulations of nanomotors, nanotubes, micelles, and custom-designed nanopores using Molecular Dynamics.**

- **Showed that**
  - **Electron tunneling can drive nano-scale motors used in nanopropellers.**
  - **Functionalized graphene-based nano-pores can serve as ionic sieves.**
  - **Nanodroplets can be dragged on the surface of carbon nanotubes.**

NERSC:

- **NAMD on Franklin; 2009 alloc: 250K hours**

PI: Petr Král, UIC



Click here

Left: Nanomotor rotates in presence of electric field; Right: two example highly-selective nanosieves – only certain ions pass across.

Phys Rev Lett., J Chem Phys,, and JACS, (2008)

U.S. DEPARTMENT OF ENERGY | Office of Science

Chemistry: Mechanism of Alzheimer's

Objective: Molecular Dynamics (MD) study of aggregation in amyloid beta (Aβ) peptide – the major species found in the brains of Alzheimer patients.

Implications: Insight into the cause of this crippling neurogenerative disease.

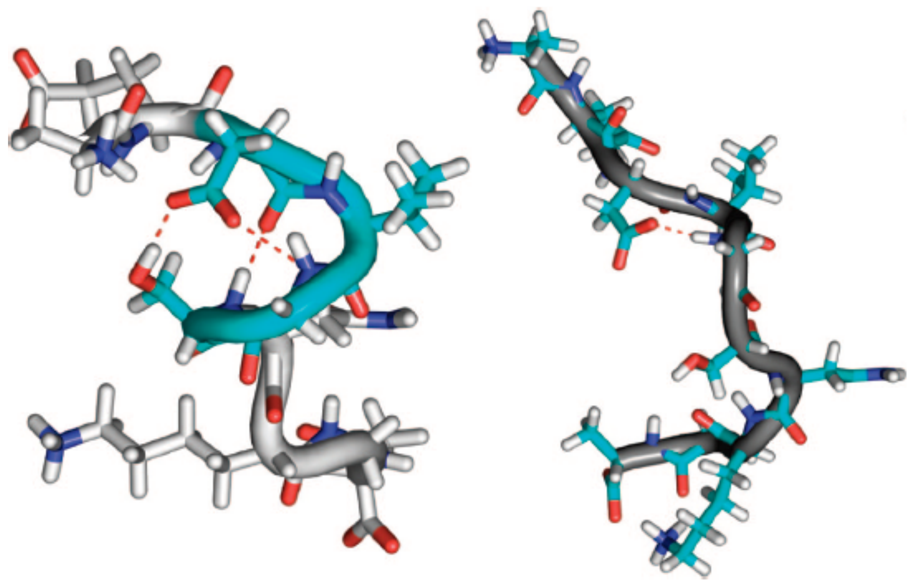
Accomplishments: Combine AMBER MD with NMR to study solution structure:

- Predict NMR coupling constants, shifts.
- Calculated ensemble structures validate well against NMR spectra.
- Shows that interplay of MD and high-quality NMR fruitful for exploring ensembles of disordered peptides and proteins.
- Use Particle Mesh Ewald + 2 replica exchange simul'ns to study ensembles.

NERSC:

- NAMD on Franklin, 1.9M hours used.

PI: T. Head-Gordon, UCB



Representative conformations of the ***Aβ***$_{21-30}$ *peptide structure showing hydrogen bonds and electrostatic interactions (dotted red).*

J. Am. Chem. Soc. 2008, 130, 6145–6158

Laboratory Scale Turbulent Lean Hydrogen Combustion

Objective: **Detailed simulations with adaptive projection code, used in tandem with experiments to explore emissions in low-swirl burners.**

Implications: **Fuel-flexible, near-zero emission gas turbines.**

Accomplishments: **Statistically stationary flames computed for variety of flow rates and fuel mixtures.**

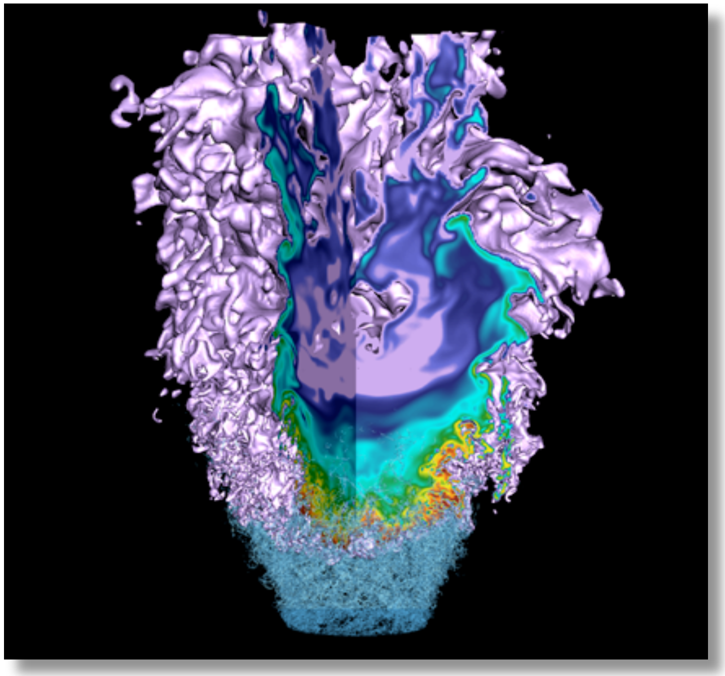
. Characterize flame shape, flow, local burning, emissions. Simulated chemical detail experimentally inaccessible, but critical for evaluation of burner scenarios.

. Domain sizes, chemical transport/kinetics detail and integrated simulation times are *orders of magnitude beyond* the reach of traditional reacting flow simulation approaches.

NERSC:

- **INCITE: 3.7M used / 4.7M alloc; 74% 4k cores+**

PI: J. Bell, LBNL



Flame radical, OH (purple surface and cutaway), along with volume rendering (grey) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. High vorticity surrounds the region of high shear generated at boundary of the annular swirling inlet.

SciDAC 2009, J. Phys Conf Ser *(in press)*

Astrophysics: Low Mach Number Flows

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Develop new low Mach number approach to study x-ray bursts (XRBs) and convection preceding ignition in Type Ia supernovae.**

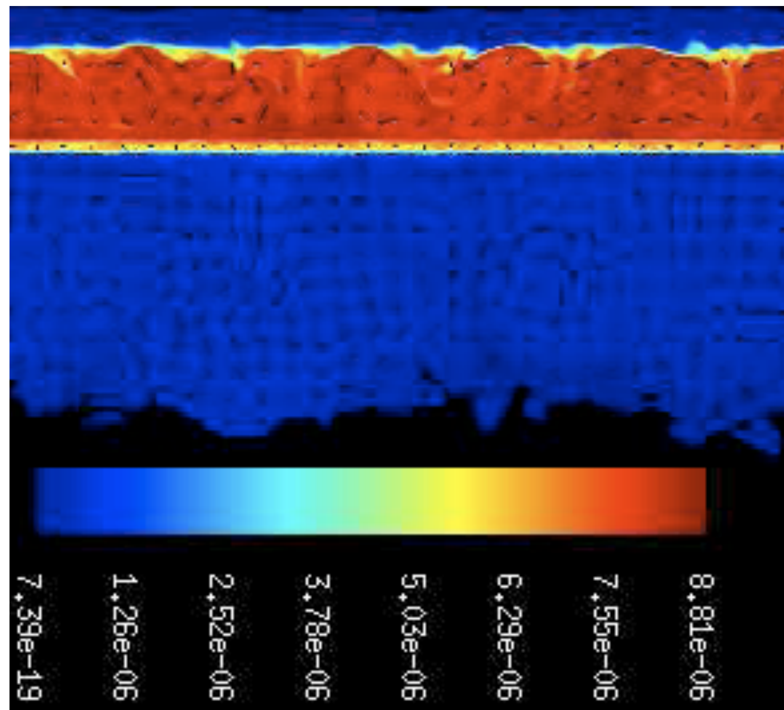
Implications: **More precise/reliable cosmological distance determination. Traditional compressible flow solvers cannot model these century-long flows.**

Accomplishments: **Implemented MAESTRO 3D hydro code for accurately, efficiently studying low-speed astrophysical flows with nuclear burn.**

- **MAESTRO with adaptive mesh refinement can calculate XRBs and model full stars in 3D, show how Type Ia supernovae ignite.**
- **Can now model low-speed astrophysical flows that are beyond the computational scope of existing compressible methods**

NERSC: **MAESTRO used for NERSC6 benchmarking & other performance studies.**

PIs: S. Woosley (UCSB), J. Bell (LBNL)



Carbon mass fraction over-plotted with velocity vectors after 22 ms of evolution for X-Ray burst convection in a 10-km neutron star using MAESTRO.

SciDAC J. Phys Conf Ser (2008)

Supernova Core-Collapse

PIs: S. Woosley (UCSB), A. Burrows (Princeton)

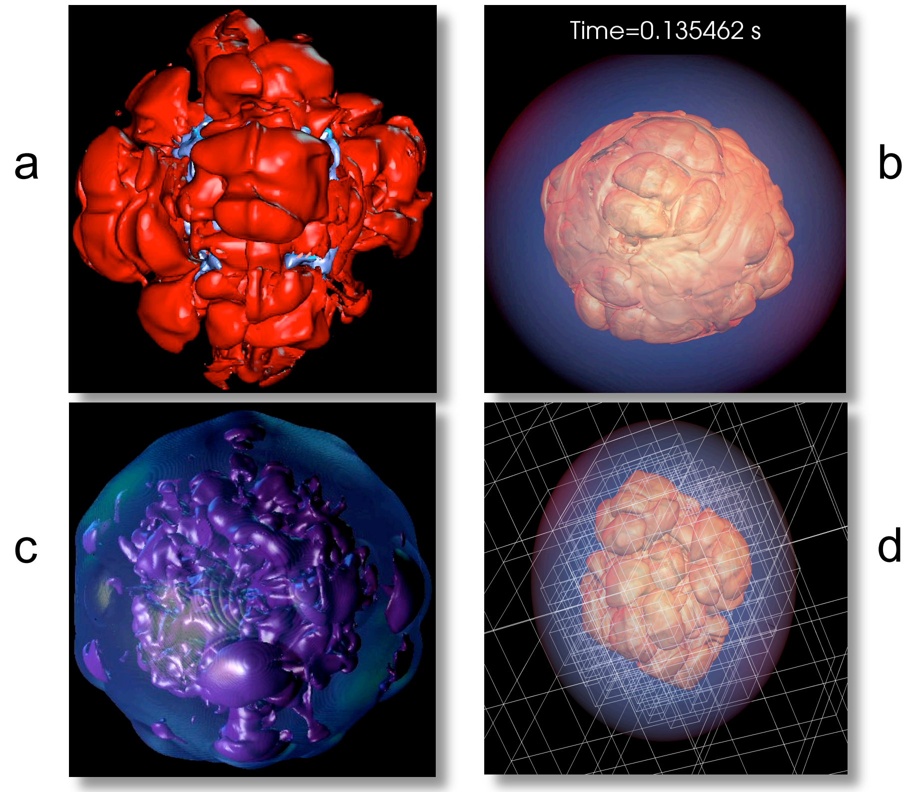
Objective: **First principles understanding of supernovae of all types, including radiation transport, spectrum formation, and nucleosynthesis.**

Implications: **Will help us confront one of the greatest mysteries in high-energy physics and astronomy -- the nature of dark energy.**

Accomplishments: **VULCAN: NERSC core collapse runs explain magnetically-driven explosions in rapidly-rotating cores.**

- **First 2.5-D, detailed-microphysics radiation-magnetohydrodynamic calculations; first time-dependent 2D rad-hydro supernova simulations with multi-group and multi-angle transport.**
- **CASTRO, new multi-dimensional, Eulerian AMR hydrodynamics code that includes stellar EOS, nuclear reaction networks, and self-gravity.**

NERSC: **2M hours alloc in 2009; 2.2M used so far, requesting additional.**



The exploding core of a massive star. a), b), and c) show morphology of selected isoentropy, isodensity contours during the blast; (d) AMR grid structure at coarser resolution levels."

Novel Material Simulations

Objective: **Electronic structure studies of complex ceramic materials with outstanding thermal & electrical properties.**

Implications: **Connection of atomic-scale characteristics with engineering mechanics and elucidation of properties not available by any other method.**

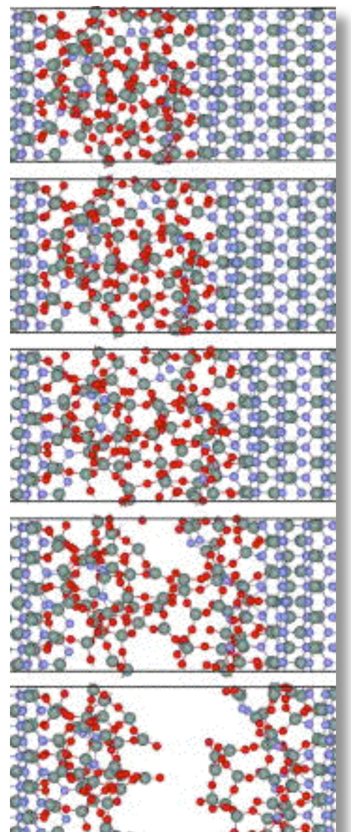
Accomplishments: **VASP DFT study of mechanical response and failure behavior of intergranular glassy films (IGFs) in Silicon Nitrides.**

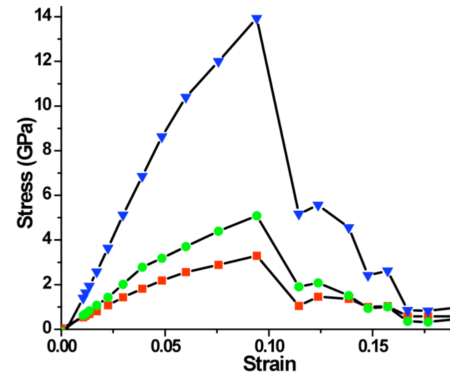
- **Stress/strain relationship explained by fundamental electronic structure of the model.**
- **May be used to guide future material designs that enhance selective properties.**

NERSC:

- **2.5M hours on Franklin used.**

PI: W. Ching, UMKC





IGF model at five different levels of strain (left) and stress vs. strain curve (right) showing a kink in the rising stress before failure, followed by a step-like post-failure behavior at higher strains.

Appl. Phys. Lett. (2009)

Chemistry: Improving Catalysis

Objective: **First-principles studies to develop better catalytic processes.**

Implications: **Improved power sources such as lithium-ion batteries, fuel cells.**

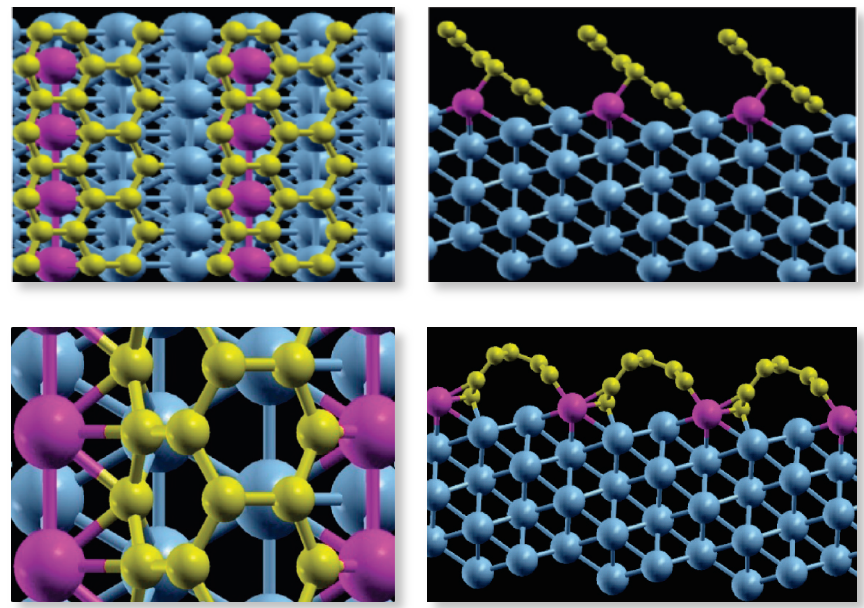
Accomplishments: **DFT studies of catalyzed single-walled carbon nano-tube growth on Cobalt nano-particles.**

- **Predict most stable adsorption sites.**
- **Carbon atoms form curved & zigzag chains in various orientations – some are likely precursors to graphene.**
- **Showed strong preference for certain metal sites.**
- **Next step is to investigate growth on chiral surfaces**

NERSC:

- **VASP / CPMD on Franklin; .7M hour alloc..**

PI: P. Balbuena, Texas A&M



Simulation showing carbon atom chains (yellow) on cobalt surfaces (blue & pink).

J. Phys. Chem. C, Sept, 2009 Cover Story

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Molecular Geochemistry

Objective: **Accurate structural studies of contaminants in solution.**

Implications: **Predict long-term viability of nuclear waste containment strategies.**

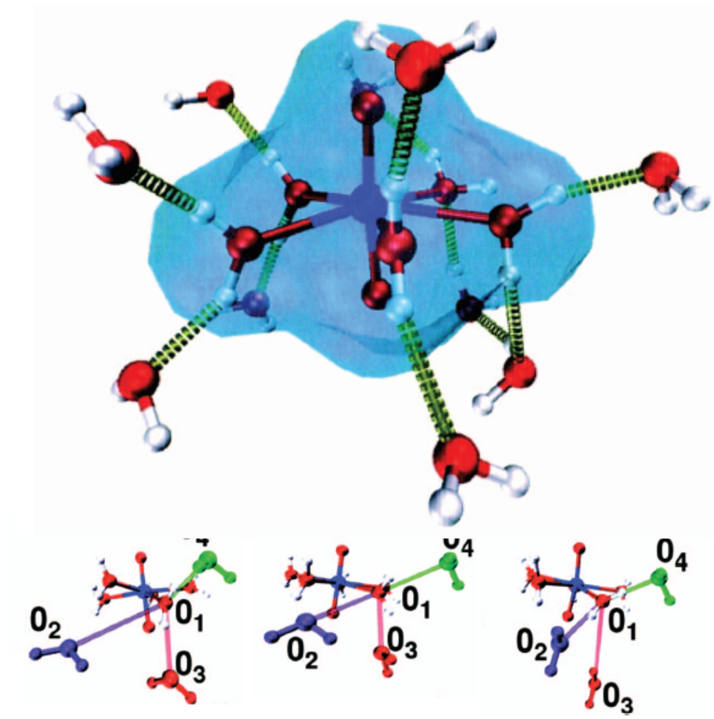
Accomplishments: **Two different NWChem *ab initio*-DFT analyses of Uranium Oxide ion (UO_2^{2+}), one with 64 H_20 molecules for 22 ps and one with 122 waters for 9 ps.**

- **Extremely-demanding simulations due to large # of H_2O molecules and long integration times.**
- **Results help explain X-Ray spectra but also reveal additional structural features.**

NERSC:

- **NWChem , Franklin, 0.6M hours. Also provides NWChem for other NERSC users.**

PIs: E. Bylaska, A. Felmy, PNNL



First-principles molecular dynamics simulation of 2nd hydration shell surrounding UO_2^{2+} with 3 intermediate dissociative structures.

J Chem Phys (2008)

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Cloud-Resolving Climate Model

Objective: Climate models that fully resolve key convective processes in clouds; ultimate goal is 1-km resolution.

Implications: Major transformation in climate/weather prediction, likely to be standard soon, just barely feasible now.

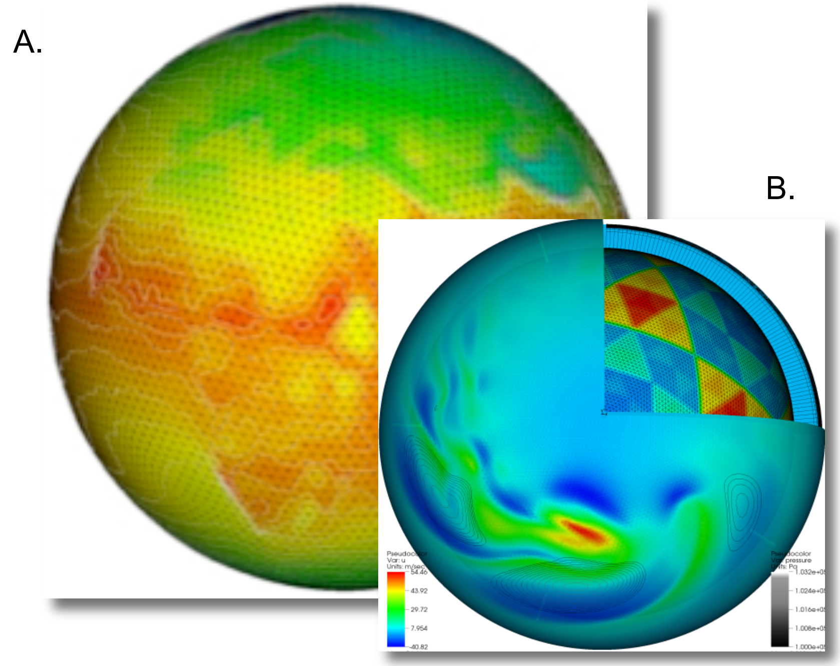
Accomplishments: Developed a coupled atmosphere-ocean-land model based on geodesic grids.

- Multigrid solver scales perfectly on 20k cores of Franklin using grid with 167M elements.
- Invited lecture at SC09.

NERSC:

- 2M hour allocation in 2009.
- NERSC/LBNL played key role in developing critical I/O code & Viz infrastructure to enable analysis of ensemble runs and icosohedral grid.

PI: D. Randall, Colo. St



A. Surface temperature showing geodesic grid.
B. Composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid.

High Energy Physics: Palomar Transient Factory

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Process, analyze & make available data from Palomar Transient Sky survey (~300 GB / night) to expose rare and fleeting cosmic events.**

Implications: **First survey dedicated solely to finding transient events.**

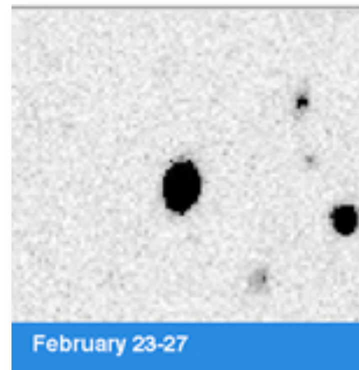
Accomplishments: **Automated software for astrometric & photometric analysis and *real-time* classification of transients.**

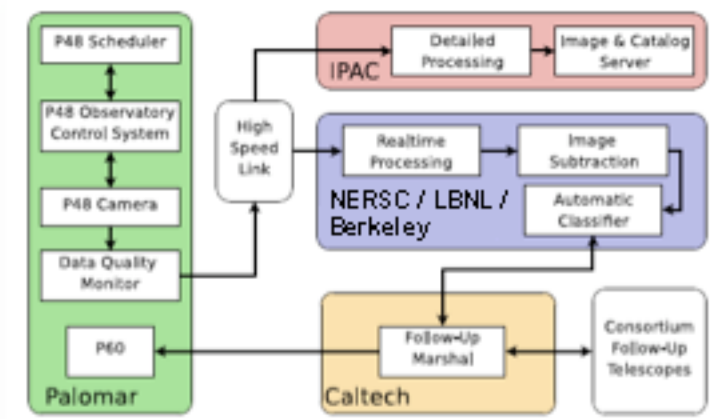
- **Analysis at NERSC is fast enough to reveal transients *as data are collected.***
- **Has *already uncovered* more than 40 supernovae explosions since Dec., 2008.**
- **Uncovering a new event about *every 12 minutes.***

NERSC:

- **40k MPP allocation + 1M HPSS in 2009; Use of NERSC NGF + gateway (next slide)**

PI: P. Nugent (LBNL)





PTF project data flow

Two manuscripts submitted to Publications of the Astronomical Society of the Pacific

Deep Sky Science Gateway

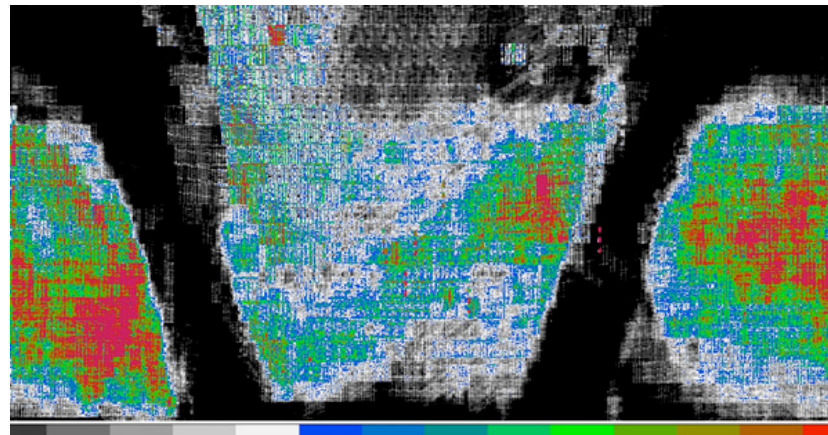
Objective: Create a richer set of compute- and data-resource interfaces for next-generation astrophysics image data, making it easier for scientists to use NERSC and creating world-wide collaborative opportunities.

Implications: Efficient, streamlined access to massive amounts of data for broad user communities.

Accomplishments: Open-source software customized to create Deep Sky database system and interface: www.deepskyproject.org

- ~ 11M 6-Mb images stored in HPSS/NGF
- DeepSky is like "Google Earth" for astronomers.
- Other NERSC gateways: GCRM (climate), Planck (Astro), Gauge Connection (QCD), VASP (chemistry/materials science).

PI: C. Aragon (NERSC)



Map of the sky as viewed from Palomar Observatory; color shows the number of times an area was observed

http://www.nersc.gov/nusers/services/Grid/SG/

Visualization Technology

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Demonstrate visualization scaling to unprecedented concurrency levels by ingesting and processing unprecedentedly large datasets.

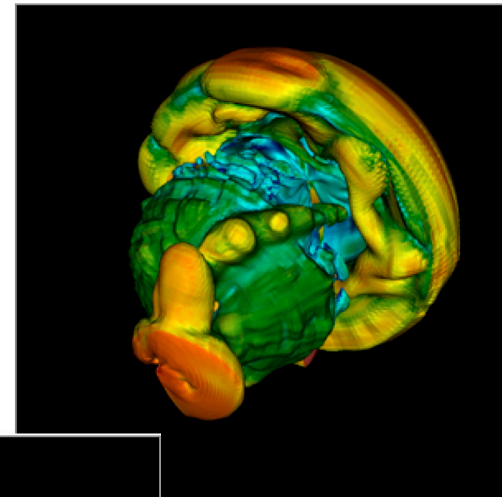
Implications: Visualization and analysis of Petascale datasets will require - and utilize - the I/O, memory, compute, and interconnect speeds of Petascale systems.

Accomplishments: Ran VisIt vis/analytics SW on 16K and 32K cores of Franklin.

- First-ever visualization of two *trillion* zone problem (TBs per scalar); data loaded in parallel.
- Demonstrated that visualization R&D has produced technology that can ingest and process tomorrow's "datasets" today.
- VisIt is the only visual data analysis SW to be part of the ASCR Joule metric.

PI: W. Bethel, NERSC

Plots show 'inverse flux factor,' the ratio of neutrino intensity to neutrino flux, from an ORNL 3D supernova simulation using CHIMERA.



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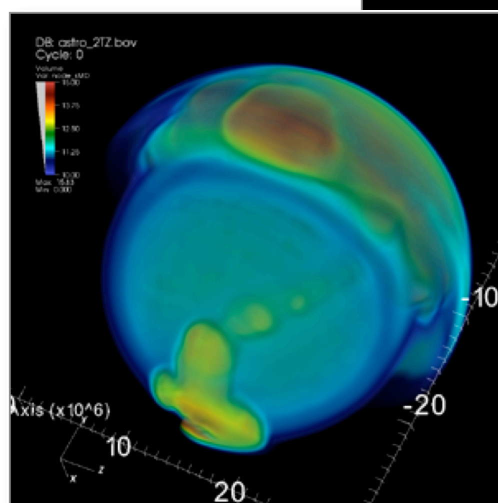

b

Isocontours (a) and volume rendering (b) of two trillion zones on 32K cores of Franklin.

U.S. DEPARTMENT OF ENERGY | Office of Science

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Catalysis for Higher Fuel Cell Efficiency

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Identify and evaluate catalytic surfaces aimed at improving the efficiency of Direct Methanol Fuel Cells (DMFCs).

Implications: Lower power, more efficient and economical DMFCs have potential applications in powering mobile phones and laptop batteries and as an alternatives to current hydrogen fuel cell technology.

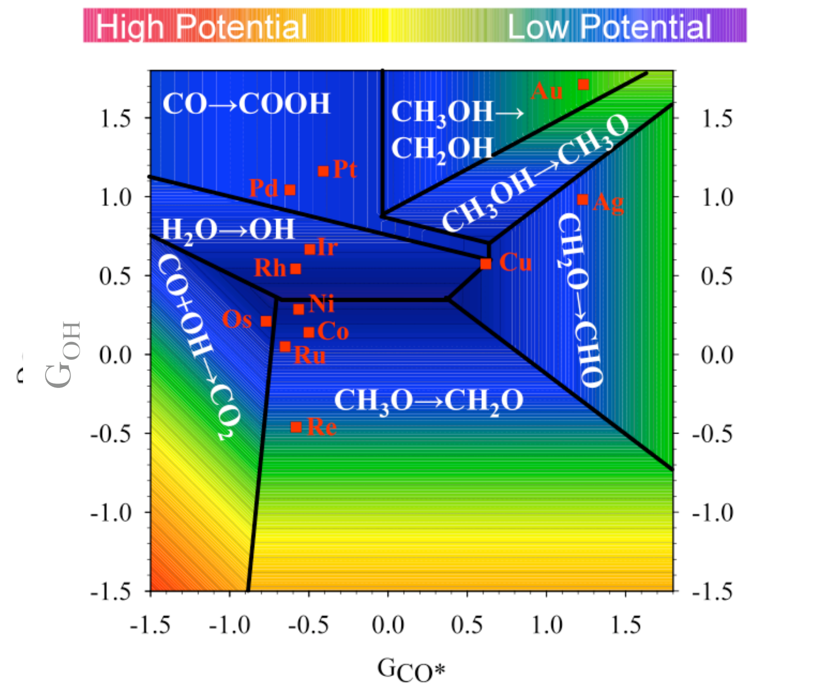
Accomplishments:

- Used DFT to develop an electrochemical model to evaluate catalytic surfaces for methanol oxidation.
- Model helps identify properties of an 'ideal' catalyst and allows screening of novel systems that may be better and cheaper than current technology.

NERSC:

- Used 700k hours thus far in 2009.
- Uses NERSC build of VASP application code.

PI: M. Mavrikakis (U.Wisc)



This figure shows the potential determining steps from the DFT calculations. It helps predict the lowest possible potential of a fuel cell, which is directly related to the efficiency of the catalyst.

Surf Sci (2008 & 2009)

HEP: Accelerator Modeling

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Use INCITE resources to help design and optimize the electron beam for LBNL next-generation Free Electron Laser.

Implications: Numerically optimizing the beam lowers cost of design / operation and improves X-ray output, helping scientific discovery in physics, material science, chemistry and bioscience.

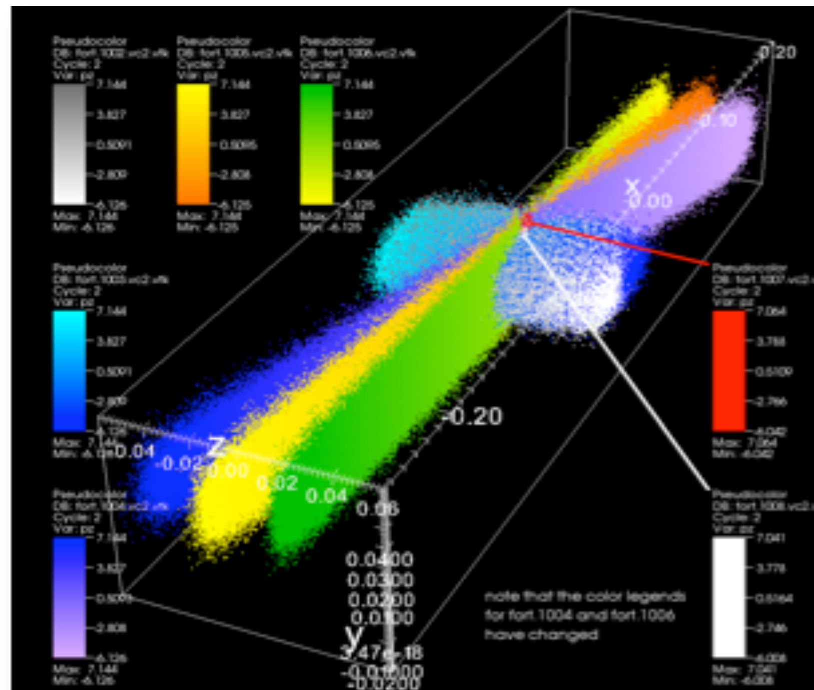
Accomplishments: Code includes self-consistent 3D space-charge effects, short-range geometry & longitudinal synchrotron radiation wakefields, and detailed RF acceleration / focusing.

- ***Billion***-particle simulation required for details of high brightness electron beams subject to microbunching instability.
- Key NERSC visualization support.

NERSC:

- 400k hours used in 2009 (~50% of allocation).
- Uses IMPACT code, part of NERSC6 test suite.

PI: J. Qiang (LBNL)



Visualization of an electron beam bending and changing orientation as it passes through a magnetic bunch compressor.

Proc. Linac08 Conference

BERKELEY LAB

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Fusion: Gyrokinetic Modeling

Objective: **Comprehensive first-principles simulation of energetic particle turbulence and transport in ITER-scale plasmas.**

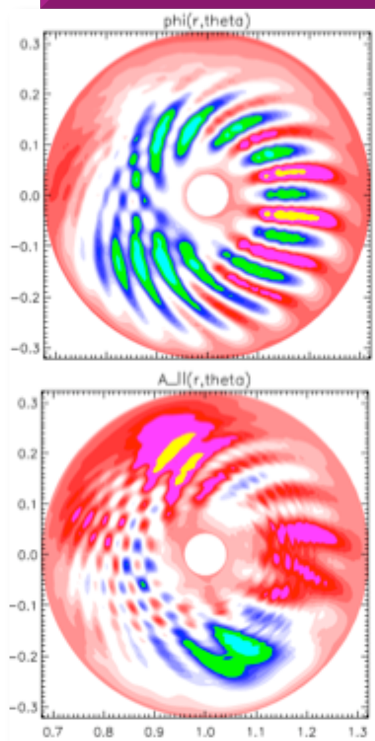
Implications: **Improved modeling of fusion systems is essential to achieving the predictive scientific understanding needed to make fusion safe and practical.**

Accomplishments: **GTC simulation successfully explains measurement of fast ion transport in General Atomics DIII-D tokamak shot.**

- **Diffusivity decreases drastically for high-energy particles due to averaging effects of large gyroradius and banana width, and fast wave-particle decorrelation.**
- **Work in preparation for 3 Fall 2009 invited talks; add'l allocation requested.**

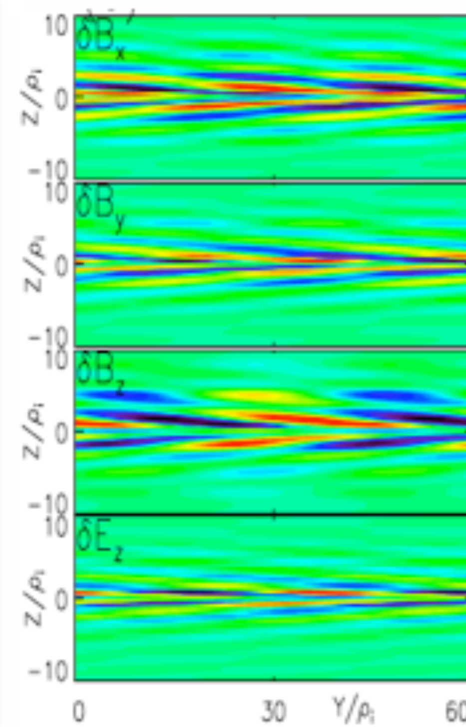
NERSC: **4M hours used in 2009; GTC part of NERSC6; 15-hour, 6,400-node run in March, 09**

PI: Z. Lin, UC Irvine



Gyrokinetic simulation with kinetic electrons using a hybrid model in GTC.

Comm Comp Phys (2009)



2-D Electromagnetic field fluctuations in a simulated plasma due to microinstabilities in the current.

Phys Rev Lett (2008)
Phys Plas. (2008)

ENERGY | Science

BERKELEY LAB

QMC Electronic Structure

PI: W. Lester, UCB

Objective: **Develop Quantum Monte Carlo (QMC) methods to stochastically solve many-body electronic structure problems.**

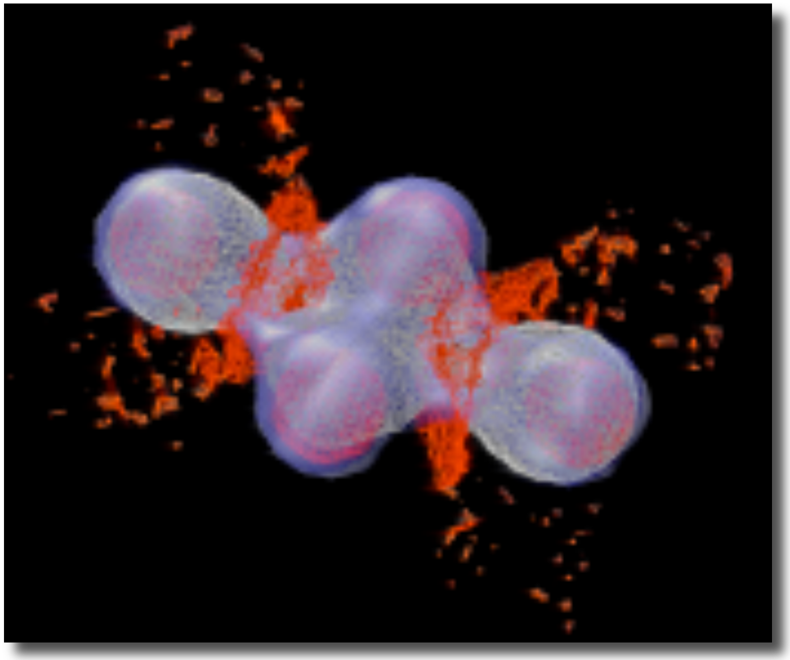
Implications: **Accurately predict or explain chemical phenomena where other methods fail or aren't applicable.**

Accomplishments: **Developed hybrid QMC / Molecular Mechanics formalism.**

- **Obtained interaction energy of a 2-water cluster treating one H_2O quantum mechanically and other classically; prelude to effort to find much sought-after electron binding energy in $(H_2O)_n$.**
- **Studied series of Li clusters in different charge states to obtain energies for cluster growth, charge, and discharge in interactions with graphene.**

NERSC:

- **ZORI scales to 32k cores on Franklin**



Cluster of four Li atoms and electron cloud (red) as calculated by ZORI on NERSC's Cray XT4

Comm Comp. Phys (2009)

Climate: Role of Eddies in Ocean Circulation

Objective: Understand deep ocean circulation and its response to an altered atmospheric composition.

Implications: Improved knowledge of CO_2 sequestration in the deep ocean and oceanic flows is crucial for understanding global climate change.

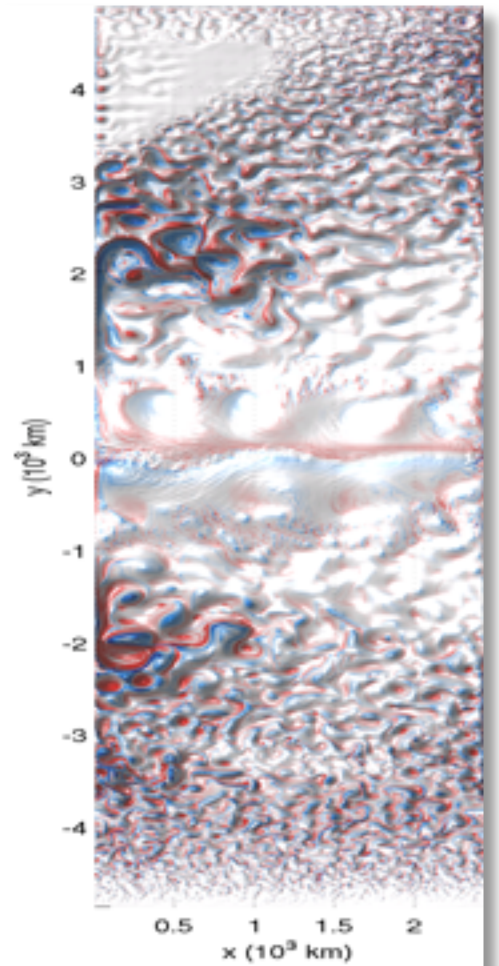
Accomplishments: First ocean model to resolve mesoscale flows over a wide range of parameters such as wind speed and surface temperature.

- Shows how dynamics of the Southern Ocean remotely control strength of meridional overturning (also known as the great ocean conveyor-belt).

NERSC:

- Completed over 15,000 simulation years using 1.6 M processor core hours, typically using 1,024 cores.

PI: P. Cessi, C. Wolfe, Scripps



A simulation capturing eddy behavior in the Southern Ocean. A key feature is the abundance of eddies away from the equator which is shown in the center of the image at y = 0.

J. Phys. Oceanography (2008)

Laser Wakefield Acceleration

Objective: **Use multi-scale simulation to understand & design laser driven plasma wakefield accelerators, supporting LOASIS experiments.**

Implications: **Offers promise of accelerators orders of magnitude smaller, less costly than current machines.**

Accomplishments: **2- & 3D PIC simulations (VORPAL) reproduce electron beam charge & energy, show physical mechanisms of acceleration.**

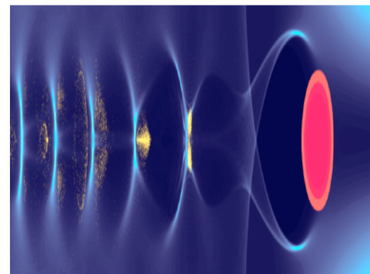
- **Used to develop new injector technologies to improve beam quality**
- **Designing a proposed 10GeV LWFA**
- **Dev'd solutions to PIC code limitations, e.g., unphysical heating & trapping.**

NERSC:

- **2.2M hours on Franklin; significant viz /analytics support; 50% of runs use ~10k cores**

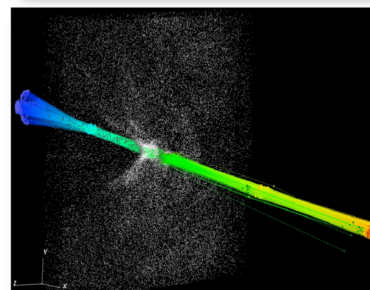
PI: C. Geddes, LBNL

(a)

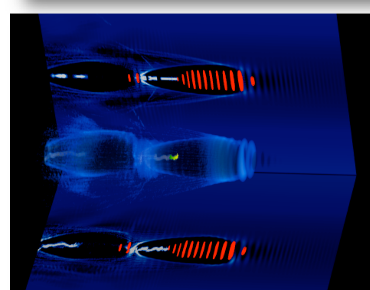


Plasma density gradient controlled injector in 2D

(b)



Particle trace of particles according to user specified criteria (momentum here; red=high)



Simulation showing 3D contours and projections of the wake (blue), laser (red), and particle bunch (yellow) in a 100 MeV LWFA

SciDAC Review Cover Story (2009)

ASCR: Adaptive Mesh Refinement

Objective: **Apply proven parallel, structured grid AMR methods to porous media flow.**

Implications: **Improved computational efficiency for subsurface flows, which typically exhibit steep concentration gradients or saturation fronts.**

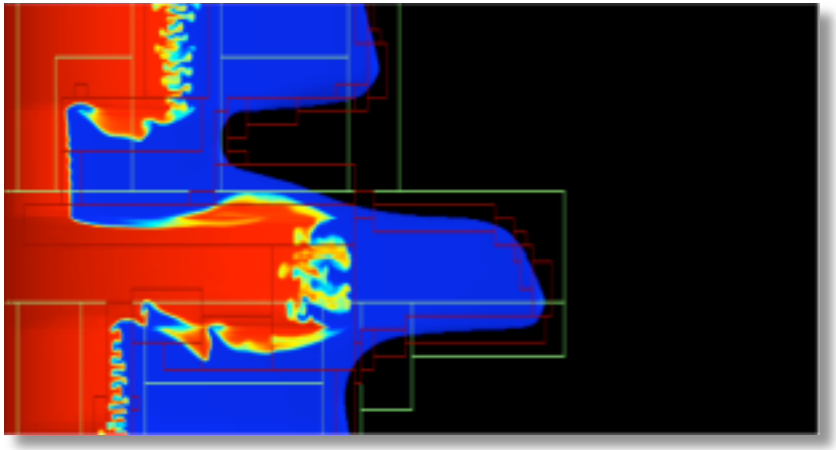
Accomplishments: **2nd-order accurate, 3-D adaptive algorithm with multiphase form of Darcy's law implemented on Franklin.**

- **Uses the well-established software framework, BoxLib, for parallelization and load-balancing.**
- **Next step is to extend the methodology to include compressibility, interphase mass transfer and thermal effects.**
- **Use in studying CO_2 storage in saline aquifers.**

NERSC:

- **1.2M Hours usage in 2009**

PI: J. Bell, LBNL



Concentration of H_20 as a function of time in a simple 3-D, 3-component, 2-phase system (2-D plane view). AMR grid is shown, 3 levels of refinement used.

Article accepted in Proc. Phil. Trans. R. Soc. A

Subsurface Biogeochemistry

***Objective*: Numerical modeling of hybrid, multi-scale subsurface biogeochemical processes.**

***Implications*: Protection of water resources, more economical extraction of fossil fuel, possible carbon dioxide sequestration**

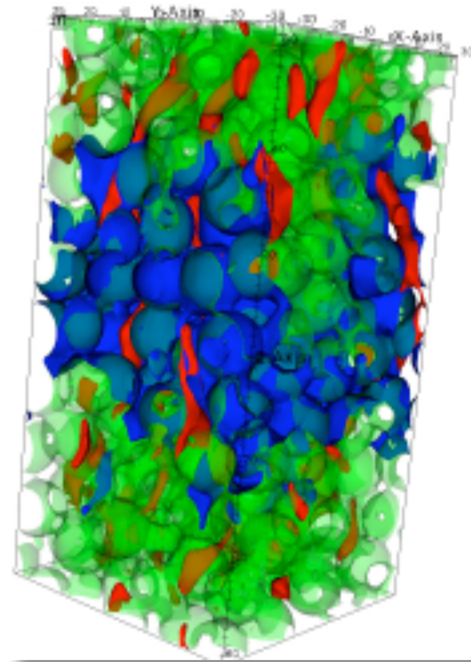
***Accomplishments:* Lagrangian Smooth Particle Hydro (SPH) methods developed, validated, for pore-scale reactive transport flow and biomass growth.**

- **Accurately estimates changes in solute concentrations due to homogenous and heterogeneous reactions during precipitation of minerals.**
- **Successful application to biofilm / biomass growth.**

NERSC:

- **.7M hour alloc.; runs using 2k-4k cores**

PI: T. Scheibe, PNNL



Visualization of a 3D SPH pore-scale simulation of fluid flow; (velocity isosurfaces in red) and solute transport (concentration isosurfaces in blue to yellow tones) in a complex pore geometry (grains indicated in green). Image generated by Bruce Palmer (PNNL) and NERSC Analytics Group.

Water Res. (2008), Intl J. High Perf Comp App (in revision, 2009)

Climate: DOE-NOAA/GFDL Collaboration

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

PI: V. Balaji, GFDL

Objective: **Early look at issues involved with resolving mesoscale features in atmospheric and ocean circulations.**

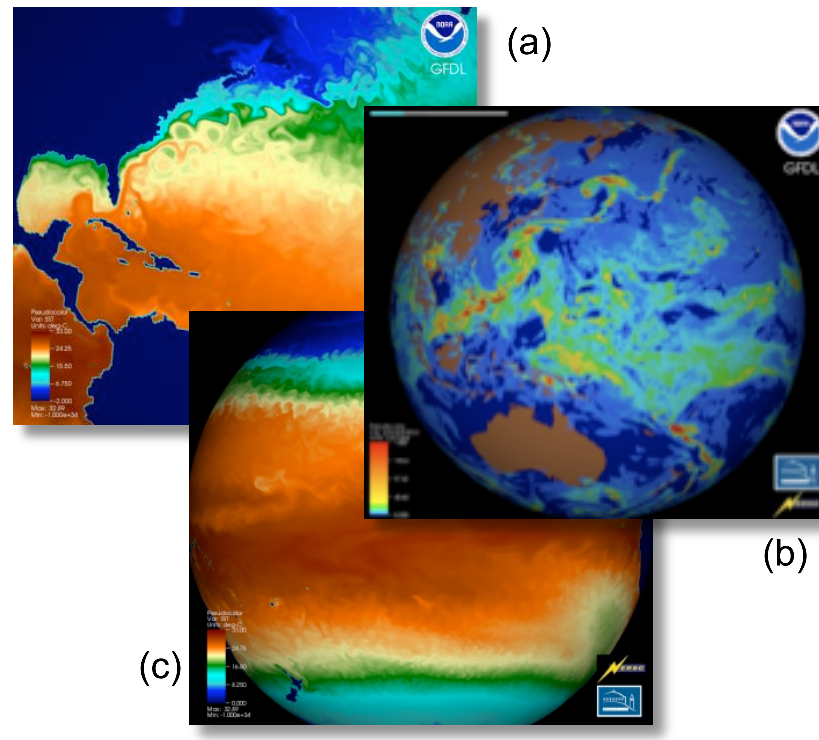
Implications: **Provide near-term insight into regional climate change; inform the design of international modeling campaigns aimed at addressing this.**

Accomplishments: **Developed global models with atmosphere resolution ≅ 5 km; ocean resolution 10 - 20 km;**

- **Based on Flexible Modeling System (FMS) w/ tri-polar or cubed-sphere grids.**
- **Experiments generate 1 - 4 TB / sim. yr.**
- **Simulation output from Franklin loaded directly into VisIt for viz., analytics.**
- **Franklin can accommodate large per-core memory needs.**

NERSC:

- **800K+ hours SC Director Award**



NERSC Analytics Team visualizations of GFDL-generated data: (a) CM2.4 sea surface temperature for North Atlantic Gulf Stream; (b) Pacific surface precipitation (c360 model); (c) Pacific surface temperature. Datasets provided by Chris Kerr (NOAA/GFDL)

Combustion: DNS of Turbulent Jet Flames

PI: J. Chen, SNL

***Objective*: Understand flame structure in future engines using lean fuels, dilute concentrations, and/or higher pressures to achieve higher combustion efficiencies.**

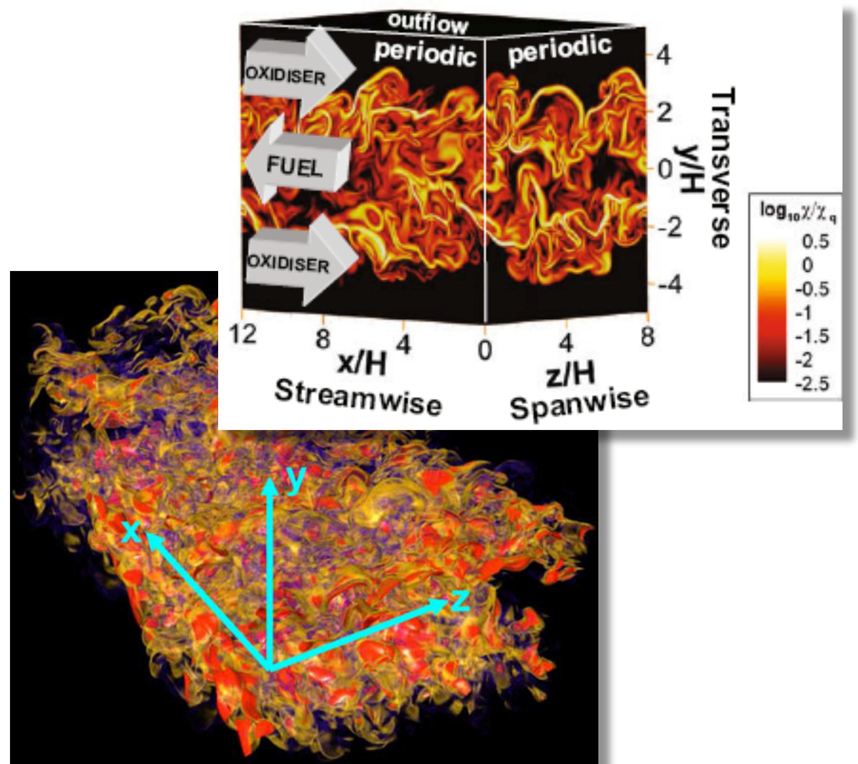
***Implications*: Can lead the nation toward the goal of increased energy efficiency and decreased emissions.**

***Accomplishments*: Direct numerical simulations (DNS) of turbulent plane CO/ H_2 jet flames using S3D to examine lower-dimensional approximations to the scalar dissipation rate – something that is vital to understand but notoriously hard to measure.**

- **Good agreement between newly-developed theoretical treatment and simulated results.**

NERSC:

- **620K alloc., jobs use up to 2,525 Franklin nodes**



Two volume renderings using the entire 500 million grid point field show the scalar dissipation rate

Proc. of the Comb. Inst. (2009)

Biology: DNA Packaging in Viruses

Objective: **Advance our knowledge of interaction of DNA with proteins and nanoparticles via Molecular Dynamics.**

Implications: **Novel designs for anti-cancer drug delivery and gene therapy. The machinery that pushes DNA into protein shells of viruses such as herpes is one of the most powerful molecular motors known.**

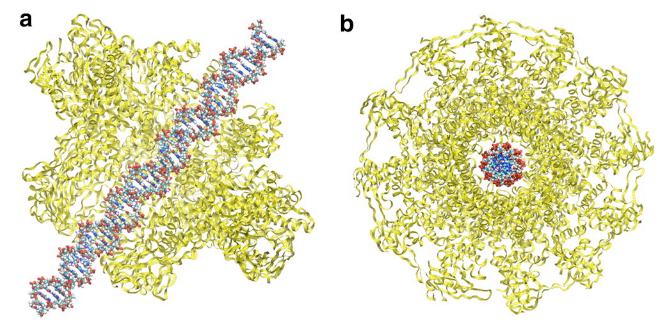
Accomplishments: **NAMD study of a model for a bacteriophage portal with a 48-base pair helix of DNA inserted.**

- **Explained mechanism of DNA import.**
- **Also developed a strategy for constructing atomic resolution dynamical ensembles of RNA molecules spanning up to millisecond timescales; applied to HIV.**

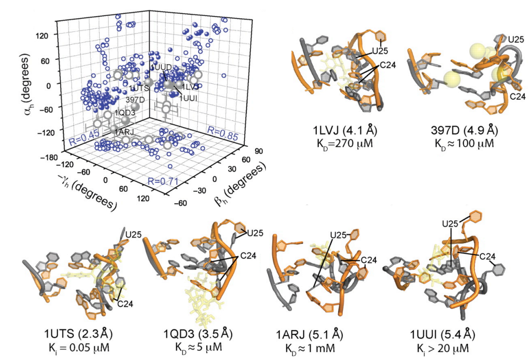
NERSC:

- **1.5M hour 2009 alloc, 1.2M used.**

PI: I. Andricioaei, UC Irvine



Side (a) and top (b) view of bacteriophage portal-DNA complex after MD equilibration. Portal protein in yellow.



Ensemble of six HIV RNA fragments studied via NAMD with a comparison of inter-helical angles in the structures shown in the upper left.

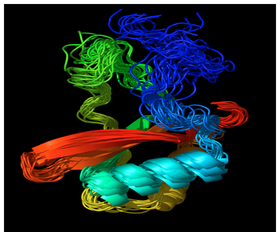
Biophys J. (2008)

Nucleic Acids Res., (2009)

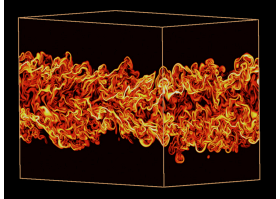
NERSC Strengths

- Enhance user *productivity*: mission is to accelerate the pace of scientific discovery.
- Infrastructure to support *all* DOE research.
- Responsive, flexible consulting and collaboration with science teams.
- SciDAC Analytics Center for Visualization.
- Versatile, easy-to-use data storage / transfer.
- High-end *production computing* to enable science, *regardless of scale.*

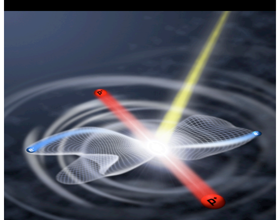
About the Cover



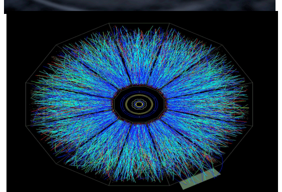
Schematic representation of 2^{o} secondary structure of native state simulation of the enzyme RuBisCO, the most abundant protein in leaves and possibly the most abundant protein on Earth. **http://www.nersc.gov/news/annual_reports/annrep05/research-news/11-proteins.html**



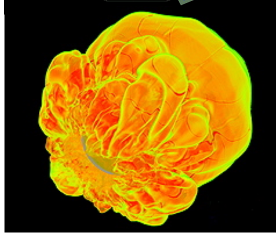
Direct Numerical Simulation of Turbulent Nonpremixed Combustion. Instantaneous isocontours of the total scalar dissipation rate field. (From E. R. Hawkes, R. Sankaran, J. C. Sutherland, and J. H. Chen, "Direct Numerical Simulation of Temporally-Evolving Plane Jet Flames with Detailed CO/H_2 Kinetics," submitted to the 31st International Symposium on Combustion, 2006.)



A hydrogen molecule hit by an energetic photon breaks apart. First-ever complete quantum mechanical solution of a system with four charged particles. W. Vanroose, F.Martín, T.N. Rescigno, and C. W. McCurdy, "Complete photo-induced breakup of the H_2 molecule as a probe of molecular electron correlation," Science **310, 1787 (2005)**



Display of a single Au + Au ion collision at an energy of 200 A-GeV, shown as an end view of the STAR detector. K. H. Ackermann et al., "Elliptic flow in Au + Au collisions at = 130 GeV," Phys. Rev. Lett. **86, 402 (2001).**



Gravitationally confined detonation mechanism from a Type 1a Supernovae Simulation by D. Lamb et al, U. Chicago, done at NERSC and LLNL