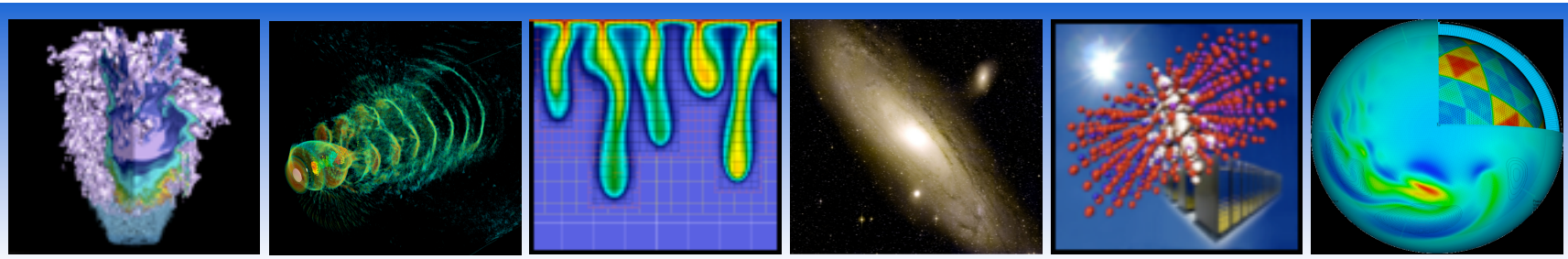

NERSC Science Highlights

A selection of scientific results produced by NERSC users.

March, 2010

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Computational Nanoscience for Energy Conversion

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

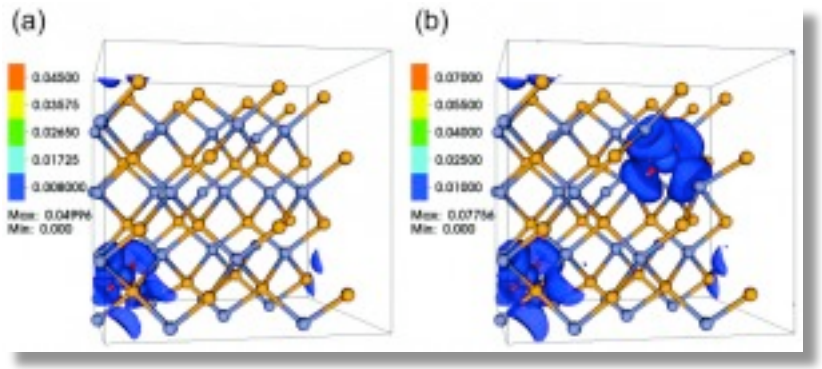
Objective: **Investigate thermoelectric efficiency of highly mismatched doped alloys using first-principles electronic structure calculations.**

Implications: **Thermoelectrics have potential for "green" energy production because of their ability to convert heat into electricity but understanding and *predicting* the capability is difficult.**

Accomplishments: **Results suggest a range of inexpensive, abundant, non-toxic materials whose electronic properties can be "tuned" for maximal thermoelectric efficiency.**

NERSC: **Uses VASP, LAMMPS, SIESTA on Franklin, Bassi, Jacquard; Project used ~1M hours in 2009 on 4-4,840 cores of Franklin, Bassi and Hopper.**

J. Wu (LBNL); J-H. Lee, J. Grossman (MIT)



Contour plots from Density Functional Theory calculations showing electronic density of states in a model highly mismatched alloy created by adding (doping) varying amounts of oxygen (3.125% in (a) and 6.25% in (b)) to a zinc (light blue) selenide (orange) compound. Oxygen atoms are surrounded by the dark-blue high density region.

Phys. Rev. Lett. 104, 016602 (2010)

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Nanoelectronic Switches

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Explain the cause of reversible binary switching in a mechanically-controlled, single-molecule junction.**

Implications: **Possible basis for a new class of switches useful for electronics. Key synergy between NERSC and LBNL Molecular Foundry.**

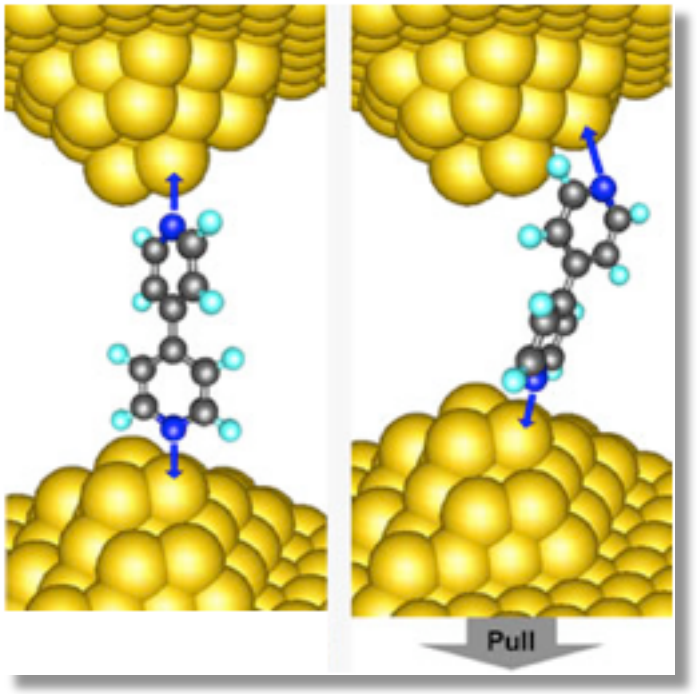
Accomplishments: **Density Functional Theory reveals the bonding mechanism in the molecule that spans the junction.**

- **Shows conductance to be directly related to degree of tilt and type of molecule.**
- **Total of 55 different junction configurations studied.**

NERSC: **High throughput and power of the NERSC resources facilitated a highly interactive back-and-forth with experimentalists.**

- **PWscf, Paratec, SCARLET Codes, typically 100-500 cores**

J. Neaton, S.Y. Quek (LBNL)



Schematics showing the molecular junction for a model nanoswitch based on a junction between gold electrodes and a bipyridine molecule that is either vertical or tilted.

Nature Nanotechnology 4, 230 - 234 (2009)

Cultural Analytics

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Apply data mining and scientific visualization to large cultural data sets to reveal trends in media and design.**

Implications: **Use of scientific analytics methods by humanists will create models for a whole new community of researchers to use high performance computing and scientific visualization / analysis.**

Accomplishments: **First-ever project to combine theoretical humanities with scientific analytical / visualization for study of large image and video datasets.**

- **Demonstrated the ability to generate numerical descriptions of, and extract patterns from, visual cultural objects.**

NERSC: **Contributed pattern recognition codes to the cultural analytics image-processing pipeline**

- **Improved workflow to allow feature extraction beyond low level & computer vision techniques.**

L. Manovich (UCSD)

Initial studies have examined variability of art, photography, and graphic design styles in Google logos (left) and Time Magazine covers (right).

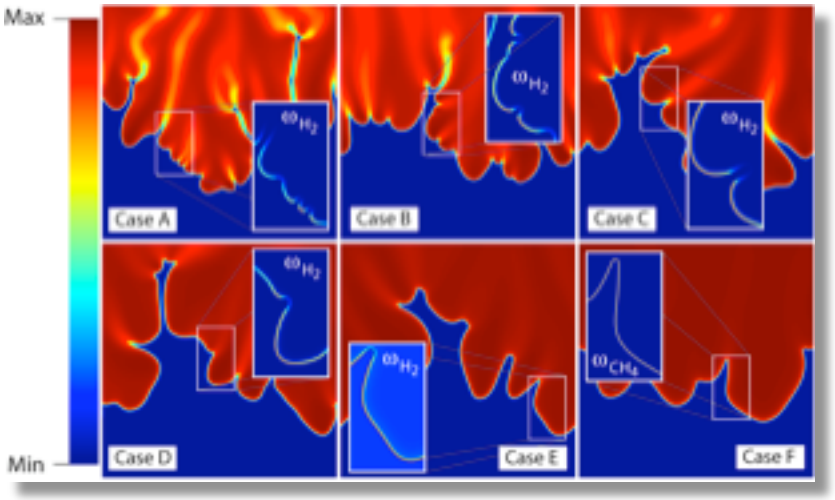
"Deep Search: The Politics of Search Beyond Google," World Information Institute (2009)

Early Hopper Science Results

***Objective*: Pre-acceptance science.**

***Implications*: Maximize DOE investment while simultaneously keeping users productive and thoroughly testing a new system.**

PI	*Affil.*	*Office*	*Project*	*Hours Repo*
Bell	LBNL	ASCR	Reacting Flows	1.6 M ***mp111***
Wilkins	OSU	BES	Spatially Complex Materials	765 K ***mp160***
Masunov	U. Cntl Florida	BES	Nonlinear optical materials	710 K ***m513***
Bhatta-charjee	U. N.H.	FES	Turbulence Reconnection	658 K ***m148***
Cheng	U. Fla	BES	High Tc materials, nanowires	484 K ***mp261***
Cheli-kowsky	U. Tx	BES	Nanomaterials	446 K ***m433***
Rubin	JGI	BER	Optimizing Genomic Storage	358 K ***m342***



*Computed snapshots of flames with six different fuel compositions from one of **four** manuscripts prepared by Bell, et al., on combustion research from computations using Hopper.*

***Accomplishments*: ~10M hours delivered, ~100 projects, ~600 users.**

- **Hopper in production on March 1**

Sudbury Neutrino Observatory Data

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

***Objective*: Archive all data (both raw and processed) for this historic project.**

***Implications*: Preserve DOE's investment in the observatory by ensuring that the unique datasets are readily available to the scientific community for decades.**

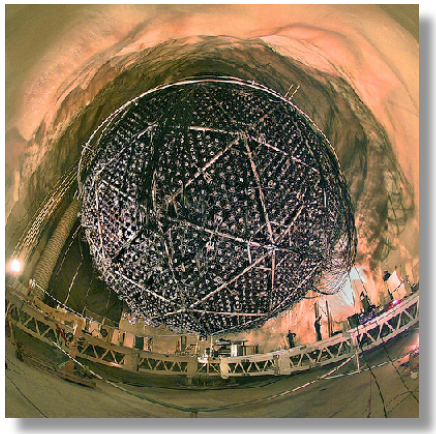
***Accomplishments:* >26 TB of data transferred to NERSC from SNO in Canada**

***NERSC:* NERSC clusters, HPSS, and staff have been supporting SNO for over 10 years.**

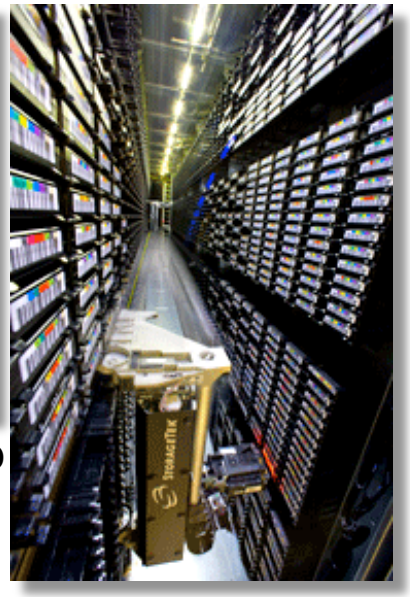
- **Considerable NERSC effort in testing the transfer speed, tuning the network, identifying packet losses, and guiding the final archive at HPSS**
- **"…the center's expertise saved us a lot of headache" – R. Martin, LBNL**

A.Poon, R. Martin (LBNL)

a



b



The SNO detector (a) and part of the NERSC HPSS tape library and robot system (b)

"NERSC has been providing great support to SNO for over a decade."
– Alan Poon, LBNL

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PHYSICAL REVIEW D 80, 012001 (2009)

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New Insights into Behavior of Water in Protein Systems

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Better understanding of protein stability and enzyme activity through molecular dynamics.**

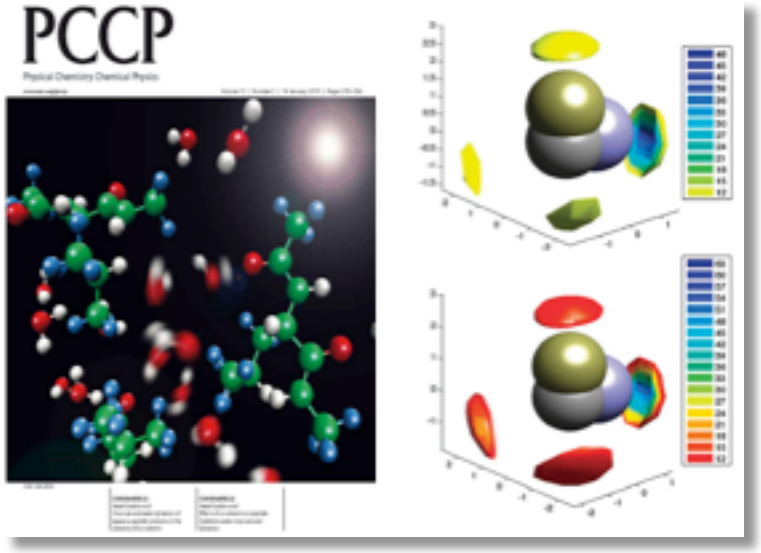
Implications: **Important because may help to develop stabilizers for protein control or design.**

Accomplishments: **Results explain why some co-solvents increase protein stability and enzyme activity while others decrease it.**

- **Protein stabilizer keeps peptide surface hydrated; protein destabilizer depletes the hydration.**
- **Cover story (3rd for THG) Physical Chemistry, Chemical Physics Journal**

- ***NERSC:*** **Uses AMBER + TINKER molecular modeling software on Franklin & Jacquard; 4-2408 cores; 250,000 MPP hours in 2009**

T. Head-Gordon, M. Johnson, C. Malardier-Jugroot (UCB)



Left*: Head-Gordon Group's Molecular dynamics simulations of a model peptide surrounded by a few in-motion water molecules on the cover of the Jan. 14, 2010 issue of Physical Chemistry Chemical Physics.*
Right*: computed spatial distribution functions of water oxygen atoms for two different co-solvents, one that stabilizes the peptide (top) and and one that destabilizes it (bottom). Simulations done at NERSC.*

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Phys. Chem. Chem. Phys., 2010, 12, 393–405

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New Type of Nonlinear Plasma Instability

***Objective*: Use magenetohydrodynamics code M3D to study large periodic instabilities called Edge Localized Modes (ELMs) in confined toroidal plasmas.**

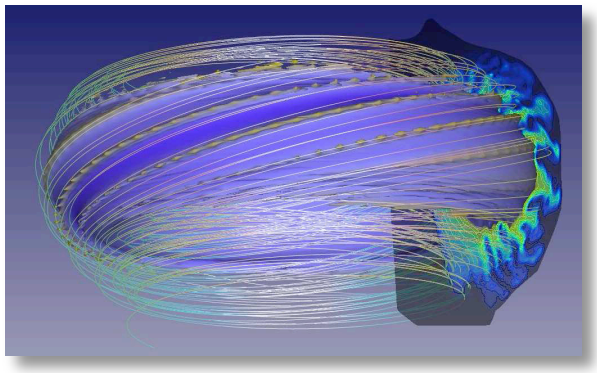
***Implications*: ELM properties have long resisted theoretical explanation; may be a constraint on the design of next generation fusion experiments such as ITER.**

***Accomplishments:* Showed that ELMs are a new class of nonlinear plasma instability.**

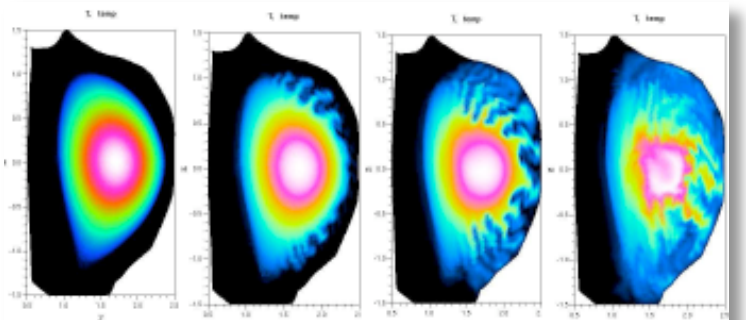
- **The instability couples to the magnetic field, drives field perturbation deep into the plasma.**
- **APS invited talk + SciDAC09**

***NERSC:* All computations, visualization done at NERSC; typically 360-768 cores; Sugiyama used 1.2M hours in 2009.**

L. Sugiyama (MIT)



Temperature surface near plasma edge shows helical, field-aligned perturbation



Time evolution of an ELM.

J. Phys: Conf. Ser. 180 (2009) 012060

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Graphene Nanostructures are Pliable

Objective: **Multiscale modeling of nanoscale systems capable of molecular transport and mechanical functions.**

Implications: **Mimic – inorganically – the behavior of proteins & cells; graphene sheets also hold promise for electronic applications and chemical separation.**

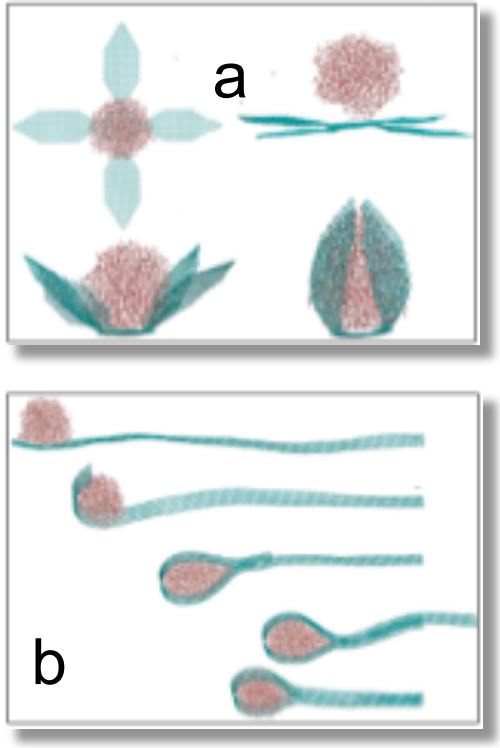
Accomplishments: **Simulations of water droplets on sheets of carbon atoms show that the sheets spontaneously fold or roll into three-dimensional shapes.**

NERSC: **Uses NERSC-provided versions of NAMD (for molecular dynamics) and SIESTA (for electronic structure);**

- **Extensive NERSC effort to provide this software so users can focus more on science.**

- **Franklin, 256-1024 cores**

P. Kral (U. Illinois/Chicago)



Molecular dynamics simulations in which nanodroplets (pink) assist and guide the rearrangement of graphene (green).

(a) *Folding of star-shaped graphene petals resembling a "meat-eating flower" and* ***(b)*** *wrapping and sliding of a graphene ribbon.*

Amer. Chem. Society Nano Letters, Vol. 9, No. 11, 2009 and Nature Vol. 462 (17) December 2009

Global Warming Potential from Halocarbon Greenhouse Gases

***Objective*: First-ever use of a global chemistry-transport model to estimate indirect global warming potential (GWP) of halocarbon gasses in the atmosphere.**

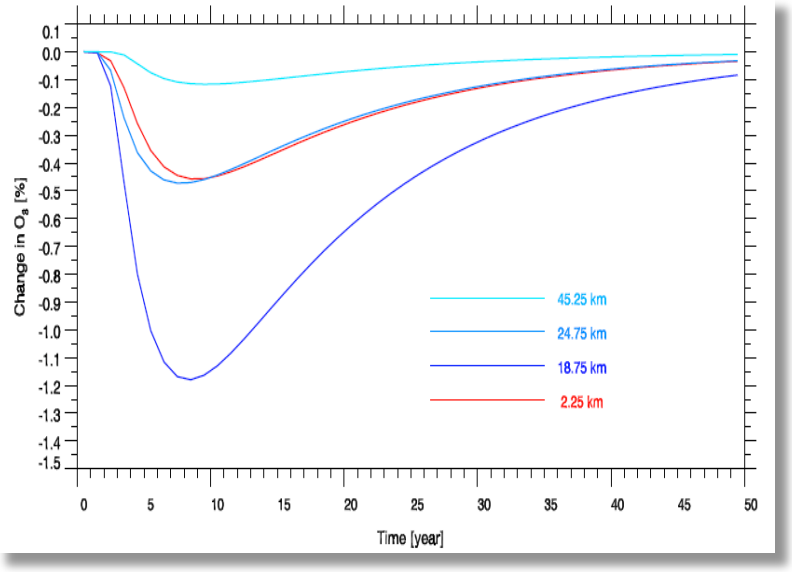
***Implications*: Halocarbons destroy ozone; ozone can both warm and cool the earth. It is critical to understand the net influence.**

***Accomplishments:* Confirms the significant importance of indirect effects on climate.**

- **Shows why GWP is a useful measure of relative climate impact; accounts for the atmospheric lifetime of greenhouse gases.**

***NERSC:* Uses GFDL "Mozart" (Model of Ozone and Related Chemical Tracers) code; up to 256 cores on Franklin & Bassi; project used ~.5 Million hours at NERSC in 2009.**

D. Wuebbles (U. Illinois)



Calculated percent change in Ozone concentration as a function of time in years at four different elevations.

Atmos. Chem. Phys., 9, 8719–8733, 2009

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Magma Dynamics

***Objective*: Simulate transport and thermodynamic properties of molten silicates at high temperature and pressure.**

***Implications*: Understanding structure, equation of state, and transport properties of materials deep inside the Earth is central to many aspects of planetary dynamics.**

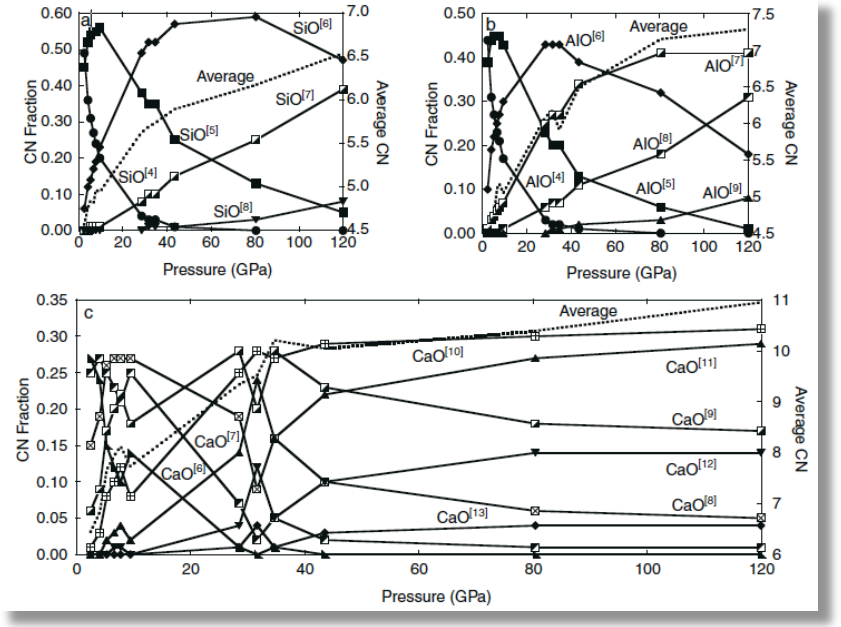
***Accomplishments:* Used Molecular Dynamics to study molten Calcium, Aluminum, and Magnesium silicates up to 6000°K and 140 GigaPascals.**

- **Viscosity and structure change dramatically with increasing pressure.**

***NERSC:* Uses LAMMPS & SIESTA on Franklin, up to 628 cores.**

- **NERSC resources allow the researchers to use more particles in the simulations; results in errors smaller than those of laboratory experiments.**

F. Spera, D. Nevins (UC SB)



Diagrams showing calculated changes in structure as a function of pressure for $CaAl_2Si_2O_8$ at a temperature of 3500°K. CN stands for "coordination number," the # of atoms connected. (c) Ca/Al; (d) Ca; (e) O

Geochimica et Cosmochimica Acta 73 (2009) 6918–6936
Amer. Mineralogist, Volume 94 (2009) 975–980

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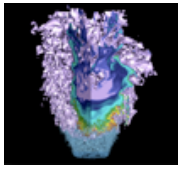
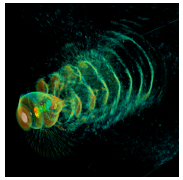
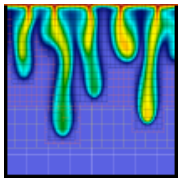
About the Cover



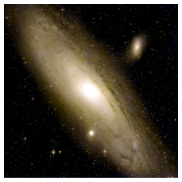
Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.



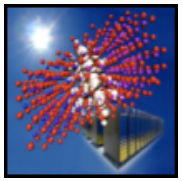
Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL.



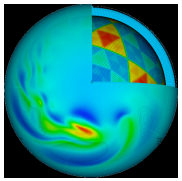
Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving the security of CO_2 storage. Image courtesy of George Pau, LBNL



False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PFT) camera in February 2009. NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod. Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



Simulation of a global cloud resolving model (GCRM). This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.