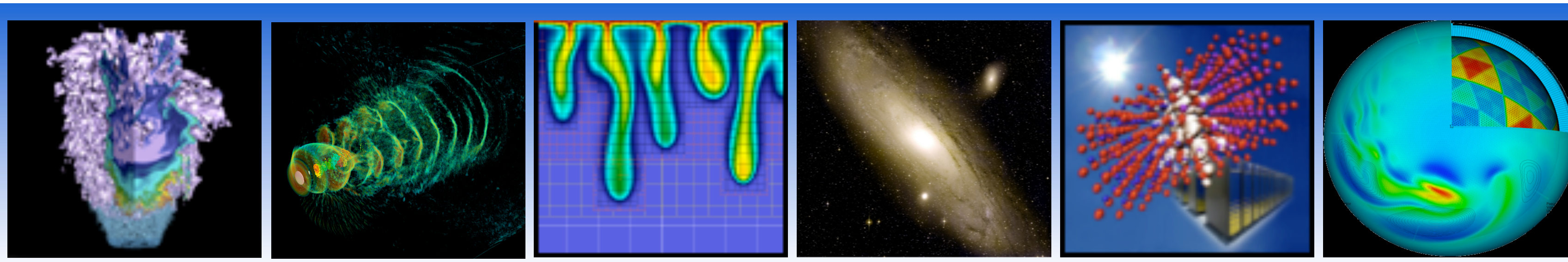


NERSC Science Highlights

December, 2009

Mitigating Global Climate Change

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Determine if global warming can still be diminished if society cuts emissions of greenhouse gases.

Implications: Provide policymakers with appropriate research so they can make informed decisions to avoid the worst impacts of climate change.

Accomplishments: CCSM used at NERSC, ORNL, ANL, & NCAR to study a century of climate conditions, two CO_2 scenarios.

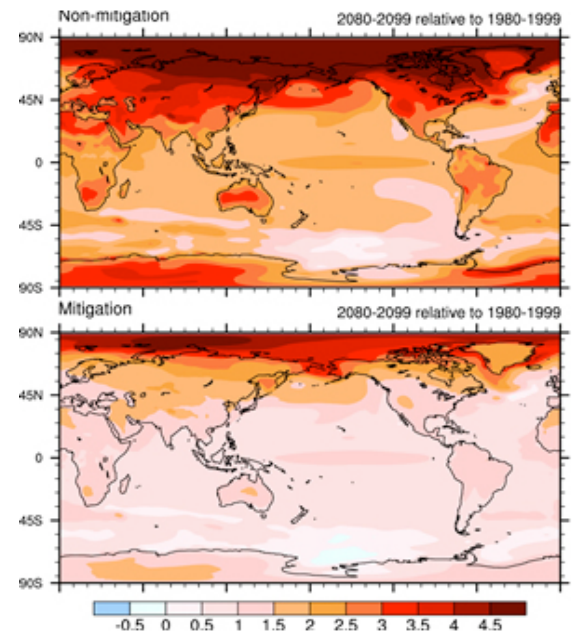
- 70% cut in emissions would save arctic ice, reduce sea level rise.

NERSC : ~2000 cores on Franklin; Part of a ~15M hour AY09 NERSC allocation;

- Newer studies at NERSC include ~20,000-yr CCSM3 T42 studies of catastrophic change in Atlantic Meridional overturning circulation.

W. Washington (NCAR)

Simulations show how average surface air temperatures could rise if greenhouse gas emissions continue to climb at current rates (top), or if emissions are cut by 70% (bottom).



Temperatures rise by <2°C across nearly all populated areas if emissions are cut but unchecked emissions could lead to warming of >3°C in those areas.

Geophys. Res. Lett. 36, 08703 (2009)

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Finding Hidden Oil / Gas Reserves

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

G. Newman, M. Commer (LBNL)

***Objective*: Apply new, highly rigorous, massively parallel, 3-D imaging techniques to create geophysical maps of hydrocarbon reservoirs in unprecedented levels of detail.**

***Implications*: New detection abilities and exploration savings by revealing where hydrocarbon deposits reside, even when covered by ocean over a mile deep and several more miles of rock below the ocean. Can also be used for locating potential sites for CO_2 sequestration.**

***Accomplishments*: Has already provided insight into complex geology of Campos Basin, a petroleum rich area near Brazil.**

***NERSC*: Code developed on Franklin.**

- **Algorithms can run on O(10,000) cores; designed to scale well beyond. Runs on Franklin routinely use 4,000-8,000 cores.**

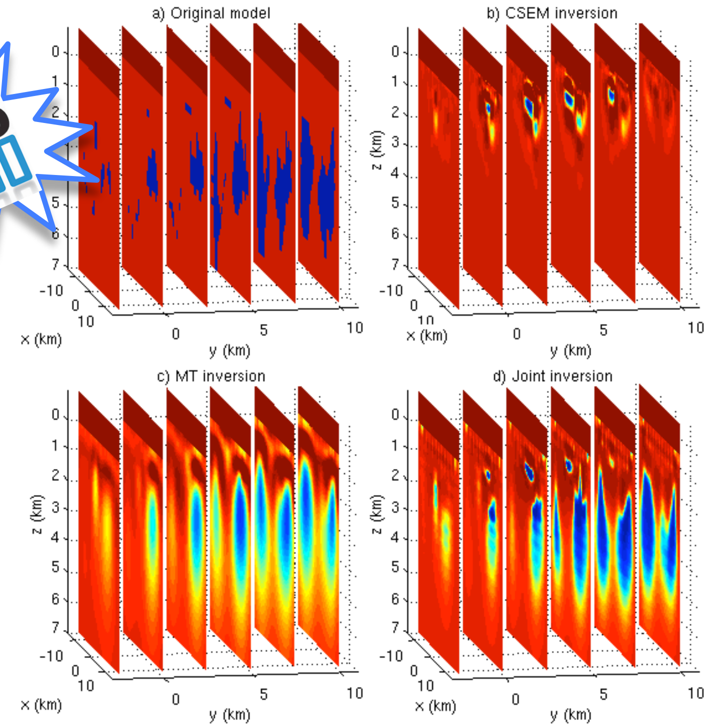

Image improvement resulting from the method. Original data (a), controlled-source electromagnetic method (CSEM) alone (b), magnetotellurics (MT) alone (c) and combined CSEM and MT (d).

http://escholarship.org/uc/item/0qh3p22m

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AMR for CO_2 Sequestration Studies

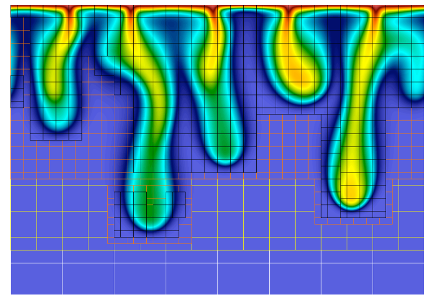
Objective: **Apply a proven, parallel, structured-grid, Adaptive Mesh Refinement (AMR) method to porous media flow to simulate diffusive convection processes involved in sequestering carbon dioxide within subsurface brine.**

Implications: **Simulations provide detailed understanding of how gravitational instability, rock heterogeneity, brine salinity, and other conditions affect the mechanism of CO_2 storage and the volume of CO_2 that can be stored.**

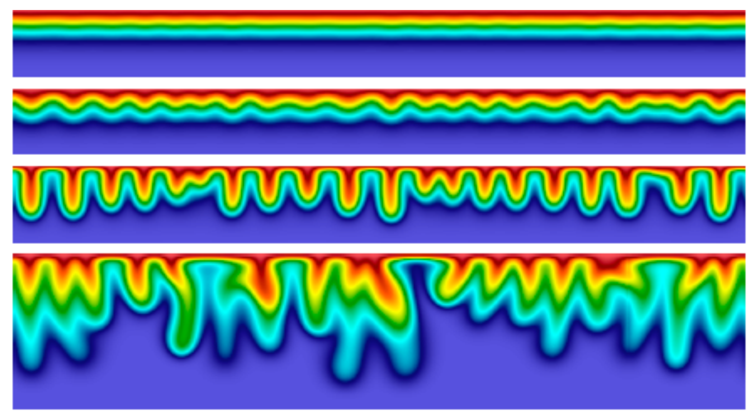
Accomplishments: **2nd-order algorithm implemented; refinement in both time and space;**

- **Simulations show chaotic nature of convection but CO_2 mass flux reaches stabilized state at time scales of interest for storage.**

Bell, Pau, Pruess, Almgren, Lijewski, Zhang (LBNL)



A snapshot of CO_2 concentration after onset of convection showing an AMR grid with 3 levels of refinement.



Density of aqueous CO_2 as a function of time (increasing from top to bottom).

Graphene as the Ultimate Membrane for Gas Separation

Objective: **Study permeability, selectivity of graphene with custom sub-nanometer pores using *ab initio* DFT and vdW DF.**

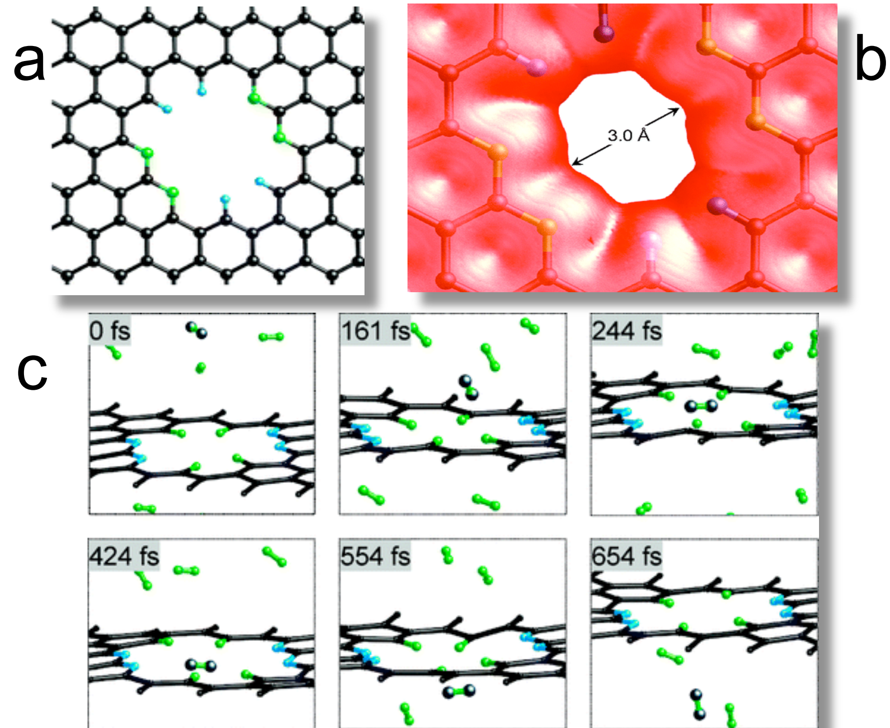
Implications: **Potentially lower energy costs for purification and production of key industrial gases such as H_2 and methane.**

Accomplishments: **Such pores exhibit extremely high selectivity, presenting a formidable barrier for CH_4 but easily surmountable for H_2.**

- **Results suggest that graphene may be superior to traditional membranes.**
- **Could have widespread impact on numerous energy and technological applications, including carbon sequestration, fuel cells and gas sensors.**

NERSC: **Franklin, VASP & ABINIT, ≤ 896 cores**

D. Jiang (PI), V. Cooper, S. Dai (ORNL)



Nitrogen-functionalized pore in graphene (a), electron density isosurface (b), and snapshots of H_2 diffusing through the pore from NERSC first principles molecular dynamics simulations.

Nano Lett., 9, 4019 (2009)

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First of Its Kind Supernova

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Objective: Develop Type Ia supernovae as tools to measure the expansion history of the Universe and explore the nature of Dark Energy.

Implications: Analysis of these supernovae is central to the success of DOE's/NASA's Joint Dark Energy Mission.

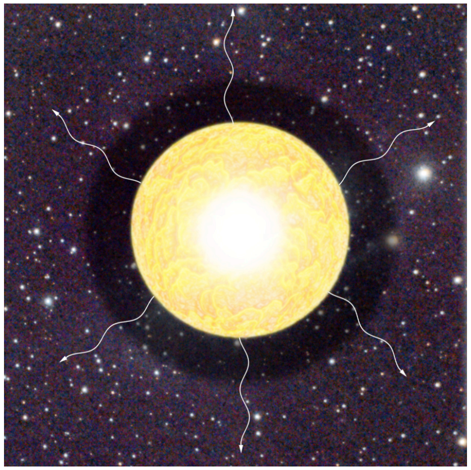
Accomplishments: Extraordinarily bright, and long-lasting supernova SN 2007bi is first unambiguous example of a "pair-instability" star, the kind that is believed to have first populated the Universe.

NERSC: NGF, PDSF, Franklin all played vital roles:

- Helped in sifting through years of data from SN Factory and other surveys.
- Used to generate synthetic spectra for comparison with the observed data.
- Spectrum code dev'd on Franklin.

HEP

G. Aldering, P. Nugent, R. Thomas (LBNL)



Schematic illustration of material ejected from SN 2007bi. Analysis carried out at NERSC using data from the Nearby Supernova Factory shows that this super-bright supernova found in a dwarf galaxy is the first confirmed example of a pair-instability supernova, the result of the partial core collapse and thermonuclear detonation of an enormously massive star, like the earliest stars in the Universe.

Nature, December 3. 2009

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New 3-D Radiation Transfer Capability

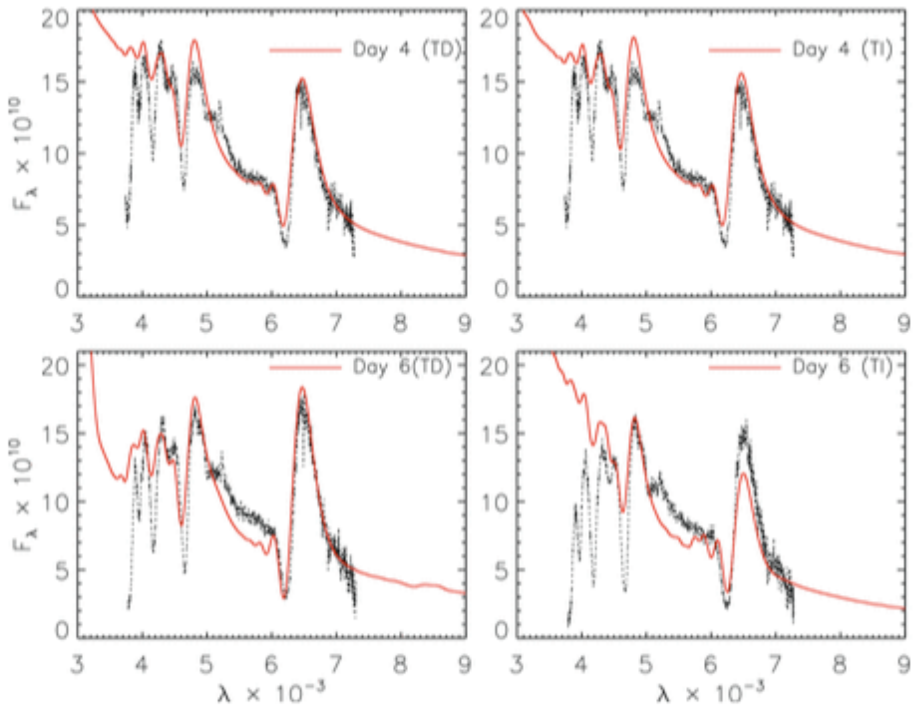
Objective: Understand detailed physics and energetics of supernovae, low- and high-mass stars, and giant planets by calculating the spectra they emit.

Implications: Because supernovae produce the stuff of which life is made, understanding which stars produce supernovae is of paramount importance.

Accomplishments: PHOENIX general purpose NLTE stellar atmosphere code now includes time-evolving, 3-D fully-relativistic radiation transfer with *arbitrary* flows.

- Parallel over both wavelength and solid angle using MPI; hierarchical domain decomposition affords very good strong and weak scaling.
- 8 papers published in 2009.

E. Baron (U. Oklahoma)



Comparison of observed spectra for SN 1987A with synthetic spectra calculated by PHOENIX from days 4 and 6 for both time-independent and time-dependent treatments.

Monthly Notices of the Royal Astronomical Society, Nov. 2009

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Restructuring Catalyst Surfaces

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

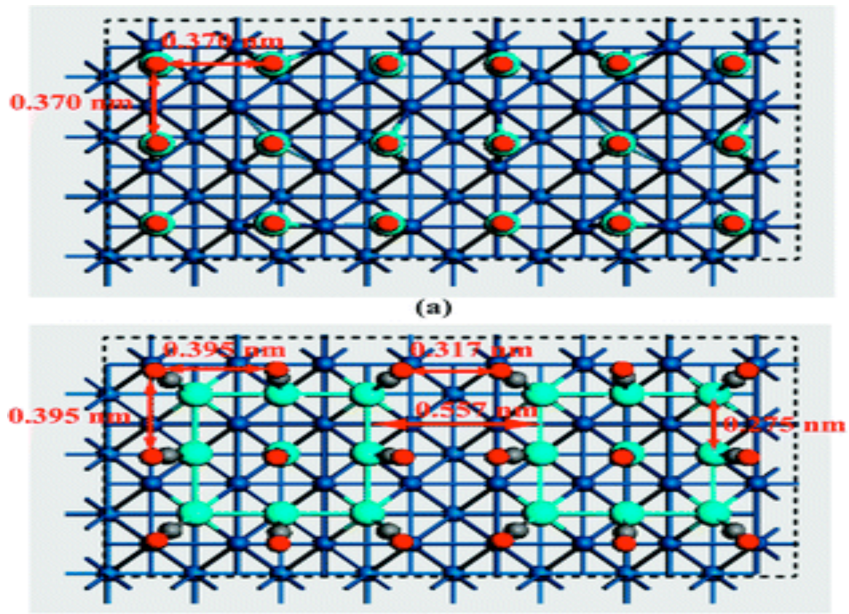
Objective: Use simulation to understand the ability of surfaces to restructure under the influence of gaseous adsorbates.

Implications: Revealing the arrangement of metal atoms that form at active sites will yield increased understanding of heterogeneous catalysis mechanisms.

Accomplishments: DFT studies at NERSC show that CO molecules bind to small Pt nanoclusters on the catalyst surface.

- The nanoclusters seem to maximize bonding of more CO molecules.
- VASP reveals the stabilization energy gained by cluster formation and suggests the atomic arrangement.
- Formation of small metallic clusters opens a new avenue for understanding catalytic activity under high pressures.

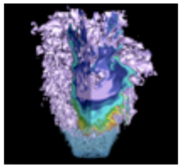
Lin-Wang Wang (LBNL)



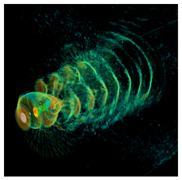
(top) Starting geometry of CO and Pt atoms. (bottom) After relaxation to minimize energy in the DFT calculation, two (3 × 3) clusters form. Dark blue circles represent Pt atoms in the slab layers; light blue circles represent Pt atoms at the surface. Red and gray circles represent oxygen and carbon atoms, respectively.

Nano Lett., 9 (5), 2167 (2009)

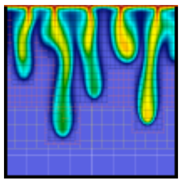
About the Cover



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.

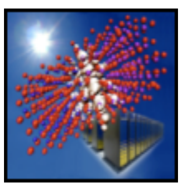


Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour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

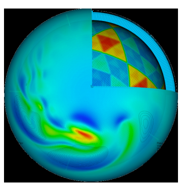


Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving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