NERSC: A Leader in Accelerating Scientific Discovery

BERKELEY LAB
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Computing Sciences

The National Energy Research Scientific Computing Center (NERSC) is the leading scientific computing facility for the U.S. Department of Energy Office of Science, serving more than 3,000 users tackling more than 400 research projects.

NERSC provides production computing services and support for all Office of Science research activities and is a world leader in accelerating scientific discovery through computation and data management. Resources are allocated to researchers from national laboratories, universities and industry through a competitive process managed by DOE.

NERSC's flagship machine is "Franklin," a 355 teraflops Cray XT4, which is used to help advance open science research in climate modeling, biology, environmental sciences, combustion, materials science, chemistry, geosciences, fusion energy, astrophysics, nuclear and high-energy physics, and other disciplines, along with scientific visualization of massive data sets. Here are several examples of NERSC's support of leading-edge science.

Simulating Laser Wakefield Particle Accelerators

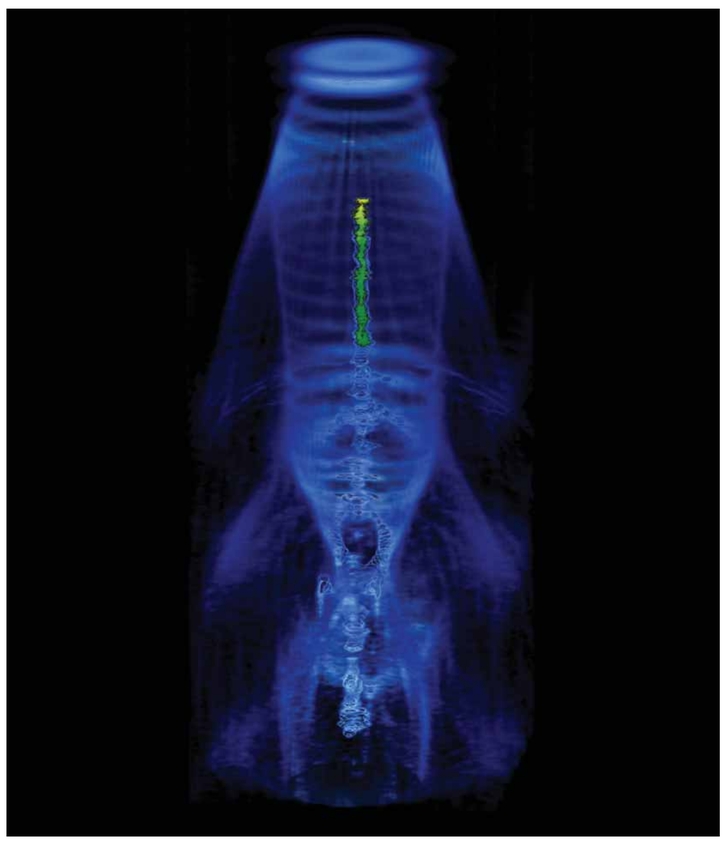
Cameron G. R. Geddes, Estelle Cormier-Michel, Eric Esarey, Carl Schroeder, Jean-Luc Vay, Wim P. Leemans (LBNL LOASIS team); David Bruhwiler, John Cary, Ben Cowan, Marc Durant, Paul Hamill, Peter Messmer, Paul Mullowney, Chet Nieter, Kevin Paul, Svetlana Shasharina, Seth Veitzer (Tech-X, Inc.); Gunther Weber, Oliver Rubel, Daniela Ushizima, Prabhat, and Wes Bethel (NERSC)

Objective
Support development of next generation accelerators and ultrafast light sources for DOE high energy physics programs by developing and using state-of-the-art particle-in-cell (PIC) simulations at unprecedented scales.

Implications
Reduced building and operating cost and improved performance for accelerators that are orders of magnitude smaller than current machines of a given energy, as well as a new generation of ultrafast beam sources.

Results
NERSC simulations over the past year helped develop new injector technologies to improve beam quality, and simulate proposed 10 GeV accelerators using new tools. Simulations have included two laser pulses colliding in a plasma to improve electron bunch injection and determine optimal parameters for experiments. The project has also improved kinetic accuracy in its models, resulting in quantitative modeling of many parameters in experiments which self-trap particles from the plasma. These kinds of studies are vital because they provide information that is otherwise inaccessible due to the lack of theoretical solutions for nonlinear 3D laser/plasma response, self consistent particle beam injection and kinetics, and other effects.

Scaling
These simulations routinely used ~4,000 Franklin cores for production VORPAL runs, and one run used over 11,000 cores.



Three-dimensional VORPAL simulation of an LBNL LOASIS experiment showing the wake (blue) and a particle bunch (green for low energy, yellow for high energy). The VORPAL code models the acceleration of particles in a laser-plasma particle accelerator capturing the self-consistent evolution of the plasma wave (wake) driven by radiation pressure from a laser pulse. Noise correction techniques nearly reproduce experimental beam properties and provide insight on how narrow energy spread bunches are formed when particles trapped by the wave are concentrated in energy due to phase slipping through the wake. Simulations such as these are used to improve future LOASIS experiments. Image courtesy of Cameron Geddes, LBNL

New Codes Yield Unprecedented Results for Computational Astrophysics

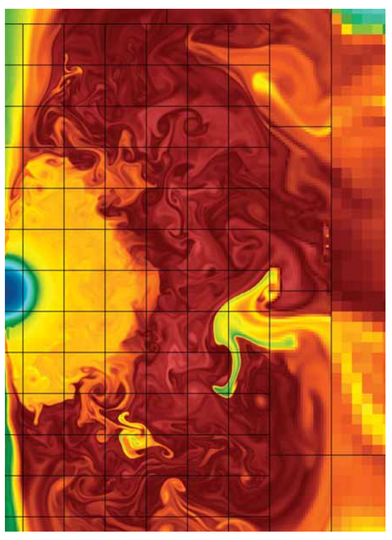
Stan Woosley (UC Santa Cruz); Adam Burrows and Jason Nordhaus (Princeton); John Bell, Andy Aspden, and Ann Almgren (LBNL)

Objective
First-principles understanding of radiation transport, spectrum formation, and nucleosynthesis in gamma-ray bursts, x-ray bursts, and supernovae of all types, in part, to aid in interpretation of experiments such as JDEM/SNAP and ground based supernova searches.

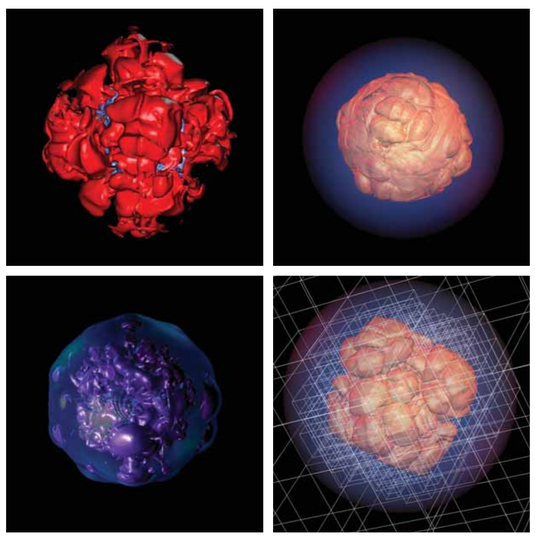
Implications
Address significant gaps in our understanding of these objects and their use as cosmological probes to confront one of the greatest mysteries in high-energy physics and astronomy today—the nature of dark energy.

Results
Two new adaptive-grid radiation-hydrodynamics packages, MAESTRO, a low Mach-number code, and CASTRO, for compressible astrophysics with stellar EOS, nuclear reaction networks, and self-gravity, have been developed using Franklin, NERSC's Cray XT4. Both codes are now used to simulate a variety of supernovae and X-ray burst phenomena. MAESTRO has allowed the first 3-D, full-star calculation of the century-long turbulent dynamics of the convective phase that precedes the final explosive runaway of a white dwarf leading up to ignition of a Type Ia supernova. CASTRO is currently being used by multiple collaborators to study Type Ia supernovae, Type II (core collapse) supernovae, pair instability supernovae, and other phenomena.

Scaling
CASTRO shows near-linear scaling to over 27,000 cores with time-explicit adaptive-grid hydrodynamics, full stellar equation of state and monopole gravity.



Adaptive grids superimposed on entropy in a Type II (core collapse) supernova, as calculated by Jason Nordhaus of Princeton University using the CASTRO code. An animation of this simulation is available at https://ccse.lbl.gov.



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

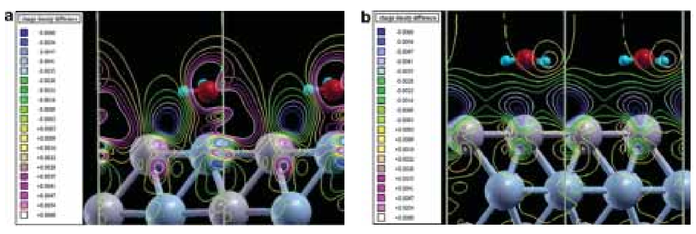
Computational Chemistry for Better Fuel Cells

Perla Balbuena (Texas A&M University)

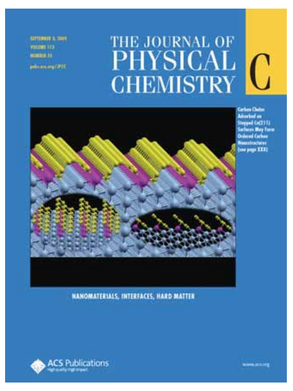
Objective
Develop a first-principles understanding of surface chemistry reaction pathways, especially for catalysis. Two key targets are the oxygen reduction reaction by platinum alloys and production of single-walled carbon nanotubes by metals such as cobalt, iron, and nickel.

Implications
Fuel cells are among the most promising next generation clean energy sources, and although platinum is an efficient catalyst for the oxygen reduction reaction that drives these devices, its low abundance and high cost limit commercial applications. An important solution is alloying Pt with cheaper metals such as Fe, Co, and Ni, the same catalysts on which carbon nanotubes, materials with extraordinary electrical and structural properties, are often produced.

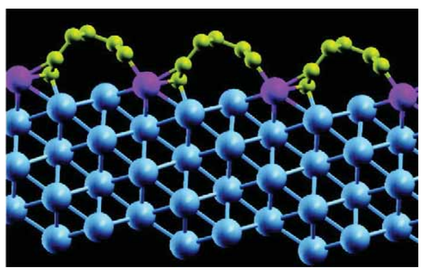
Results
New methods for stability analysis of metal nanoparticle catalysts in acid medium have been developed. These new computational methods allow evaluation of the effectiveness of many different alloy surfaces as fuel cell cathodes. A density functional theory (DFT) study of surface atomic distribution and water adsorption on Pt–Co alloys showed that the formation of a Pt monolayer is thermodynamically favored on these surfaces. Such a monolayer has better reactivity properties and is more stable against dissolution in acid medium that pure Pt(111) surfaces. This work also found that water does not spontaneously dissociate on the ordered and segregated surfaces, and especially on Pt-monolayers, buckling of Pt atoms is much smaller than that found on pure Pt surfaces. Both findings are optimistic results for developing less-expensive aqueous metal catalysts for fuel cells.



Contour plot of the DFT-computed charge density difference projected on the yz plane of (a) water located on top of cobalt in a PtCo catalyst alloy (b) water located on top of pure platinum. Grey: Pt and Blue: Co. The plots show the difference between the charge density of the total system and those of a clean metal slab and a water molecule and they reveal charge density increase (yellow and pink contours) in the bonding region between cobalt and the water molecule but a bonding density decrease between water and platinum.



Professor Balbuena's simulations of adsorption of carbon on cobalt surfaces, a study related to a technique for producing single-walled carbon nanotubes using NERSC's Cray XT4 supercomputer, were recently the cover feature in the American Chemical Society's Journal of Physical Chemistry (September, 2009).



Views of some of the carbon structures (yellow) that form close to the cobalt surface (purple, blue) in simulations of carbon adsorption. Prof. Balbuena's work suggests that the structures in DFT simulations may be single wall carbon nanotube predecessors.

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