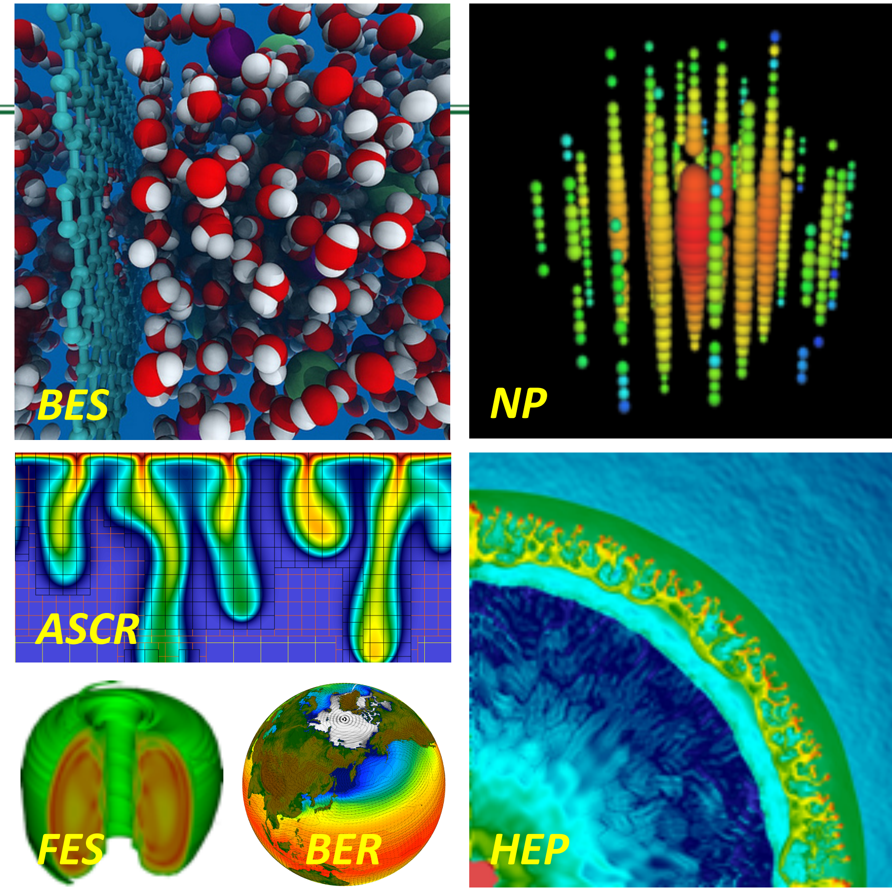
NERSC Science Highlights



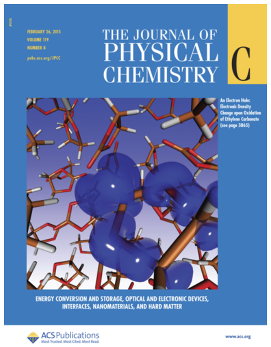
NERSC

Selected User Accomplishments

March 2015

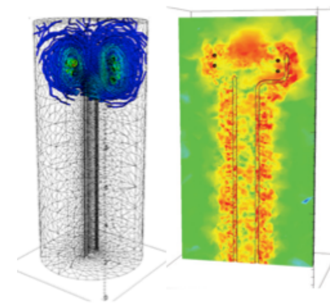
U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC User Science Highlights

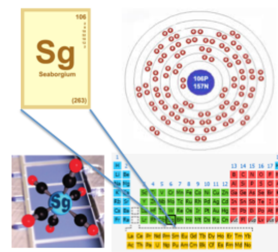


Chemistry
New theoretical method allows accurate but reduced cost multiscale modeling; yields key results in battery research
(T. Barnes, T. Miller, Caltech)

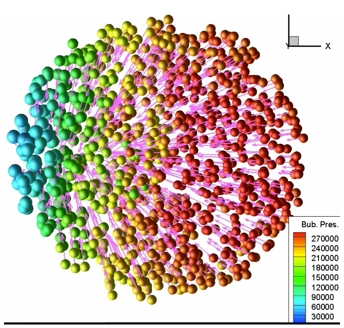
Fusion
Modeling at NERSC is helping to optimize the operation of another DOE facility
(S. Veltzer, Tech-X, Inc.)



Climate
Climate change effects on the wind turbine industry are being evaluated at NERSC
(**S. Capp, Vertum.com)**

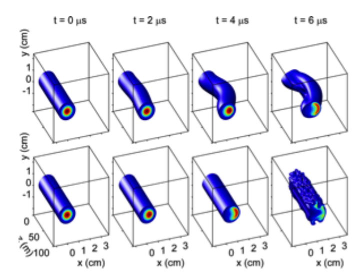


Nuclear Physics
Theoretical investigation of element 106 predicts stability of organometallic molecule of seaborgium
(G. Malli, Simon Fraser U.)



Multiscale Modeling
A numerical model accurately captures flow dynamics of microbubbles that can help and/or hinder industrial machinery.
(J. Ma, DynaFlow, Inc.)

Fusion
Simulations under conditions relevant to the ITER device describe unwelcome plasma edge electromagnetic effects
(W. Lee, UCSD)



Boosting Battery Research

Scientific Achievement

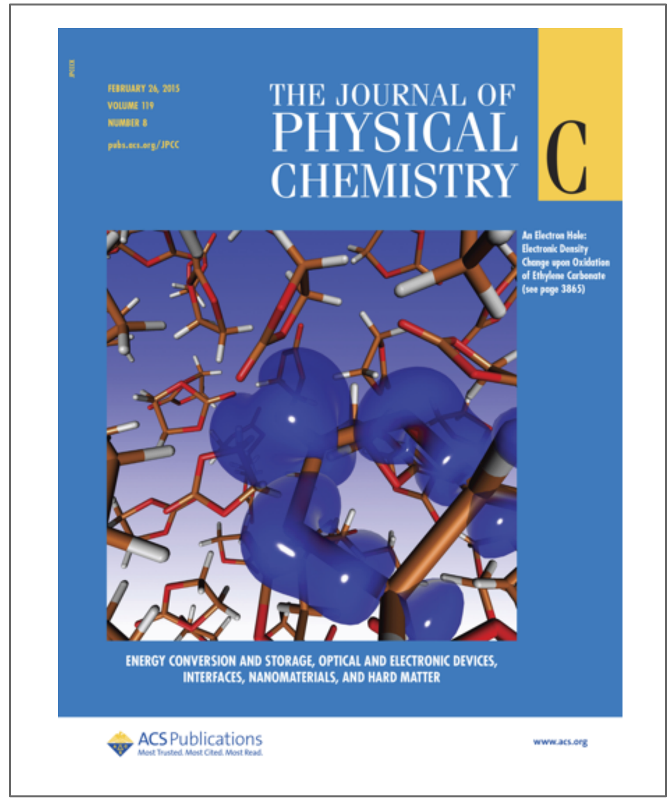
Development, validation, and application of a new theoretical chemistry method that allows accurate but reduced-cost multiscale modeling

Significance and Impact

The new method provided key insight regarding a central challenge in lithium-ion battery research: control of electrolyte decomposition

Research Details

- The new "wave function-in-DFT" embedding approach enables accurate calculation of ionization energy for individual solvent molecules at high accuracy while still accounting for bulk solvent effects using a combination of DFT and molecular mechanics interactions.
- Will be included in commercial software product
- New method used to demonstrate that the known properties of two common battery solvents are governed by fundamentally different intermolecular interactions
- Showed why less accurate methods can fail and why it's essential to treat solvent interactions accurately



On the Cover: A plot showing the oxidized electron hole density distribution in two-molecules of ethylene carbonate, which is an electrolyte commonly used in lithium batteries and is known to decompose with time, affecting battery longevity. This work helped explain the chemistry of the decomposition process.

T. Barnes, T. Miller, et al., J. Phys. Chem. C., 2015, 119 (8), pp 3865–3880. Cover

Work was performed at Caltech using NERSC

Supercomputers and the Future of Wind Energy

Scientific Achievement

Success in simulations to assess impact of complex terrain on wind turbine efficiency is now leading to assessment of climate change and lightening effects on wind power production and revenue.

Significance and Impact

Electric utilities are keenly interested in evaluating the effects of climate change and extreme weather on wind energy.

Research Details

- Uses the WRF code to solve a 4D model of the atmosphere, including all basic dynamics and energy equations, while allowing for targeted parameterizations and interaction with the land and water bodies.
- NERSC resources allow evaluation of the sensitivity of the model results to different land surface types, atmospheric datasets and other forcings both internal and external to the model.

This work has been using **4-D next-generation mesoscale numerical weather simulations** that model complex atmospheric data resolved to local wind farm scales. This will allow for optimal turbine site selection and evaluating the true climate change effects to wind energy.

Capps and Whiteman, 15th Annual WRF Users' Workshop

Work was performed at LBNL using NERSC

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VertumPartners

3-D Simulation of Intense Bubble Formation

Scientific Achievement

A numerical model accurately captures flow dynamics of microbubble clouds in water.

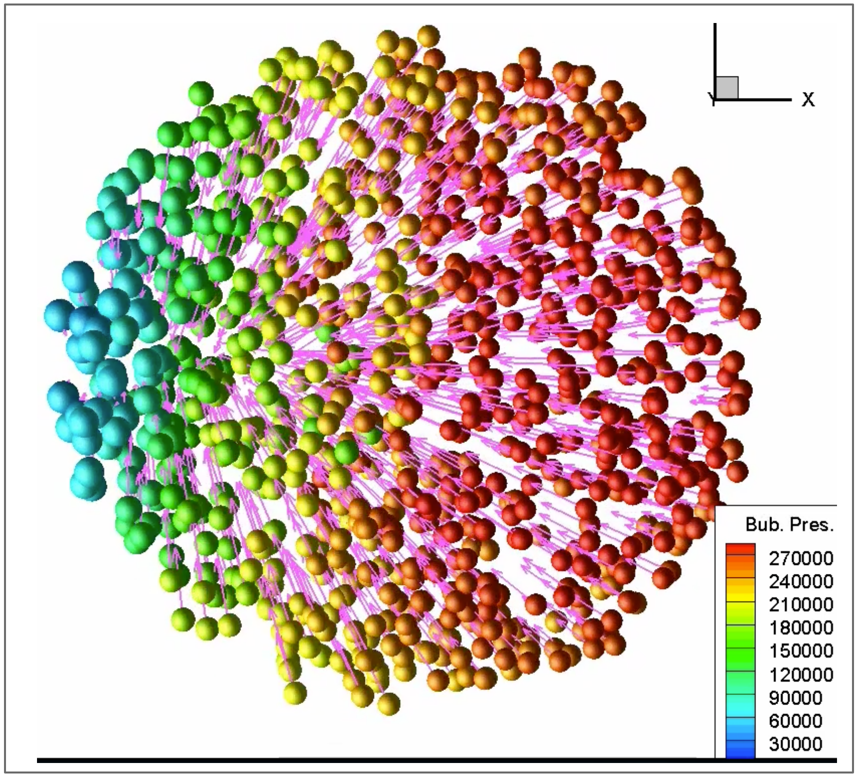
Significance and Impact

Bubbly flow plays an important role in many industrial applications: it can cause cavitation leading to efficiency loss in turbomachinery but can be exploited to enhance cutting, drilling, cleaning, and chemical manufacturing.

Research Details

- The model solves the Navier–Stokes equations using Eulerian grids with a time and space varying density over the two-phase bubble/water medium.
- Challenging multiscale physics ranging from micron-scale individual bubbles to meter-scale flow fields
- The simulations show how to "tune" the bubble cloud characteristics and initial pressure so as to generate very high cavitation forces that could be used for beneficial purposes.

Jingsen Ma, and others:
Chemical Engineering Science 128(2015)64–81;
Journal of Fluids Engineering April 2015, Vol. 137 / 041301-1



Snapshot from simulation of a circular bubble cloud driven by an initial pressure wave showing color-code bubble pressure and (pink) velocity vectors. The simulation revealed that the cloud has a natural oscillation frequency that, if matched to the natural frequency of the initial pressure wave, can create very high pressures with peak values an order of magnitude larger than the initial pressure.

Work was performed at Dynaflow, Inc. using NERSC & other resources

NERSC Supercomputer Helps Optimize DOE Facility

Scientific Achievement

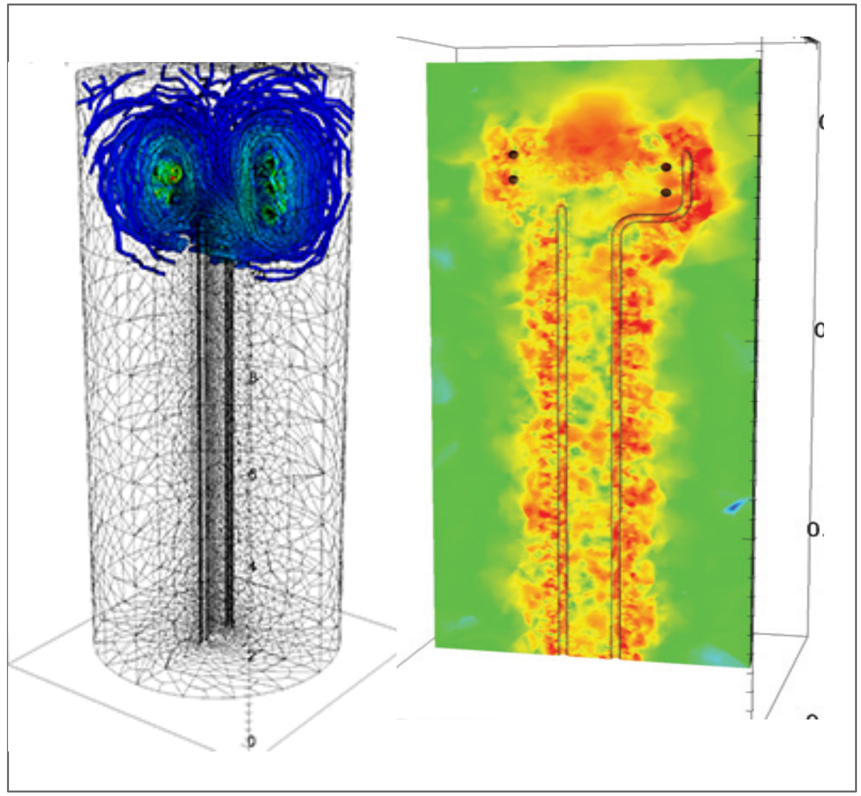
Numerical modeling of the Spallation Neutron Source (SNS) ion generator is helping to optimize designs that will reduce antenna failure and improve ion source performance.

Significance and Impact

SNS is a one-of-a-kind facility providing pulsed neutron beams for science and industry but its ion-producing antennas often fail due to plasma heating that destroys protective insulating coatings.

Research Details

- The magnetohydrodynamic fluid simulation included plasma models and complex embedded boundaries representing the rf antenna with a fully unstructured 3-D computational mesh
- Used the USIM model, which scales well, under both strong and weak scaling, on Hopper



Snapshot from simulation of SNS rf antenna. Right: Magnetic field and unstructured computational mesh structure. Left: total plasma velocity for the two-temperature magnetohydrodynamic model after 375 rf periods showing increased plasma velocity near the antenna bends.

S. Veitzer, P. Stoltz, and others:
Fourth International Symposium on Negative Ions, Beams and Sources
AIP Conf. Proc. 1655, 030004-1–030004-7; doi: 10.1063/1.491643

Work was performed at Tech-X, Inc. using NERSC

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TECH-X SIMULATIONS EMPOWERING YOUR INNOVATIONS

Superheavy Element Yields to NERSC Supercomputers

Scientific Achievement

Computation predicts the stability of a trans-actinide compound with metal-carbon bonds: seaborgium hexacarbonyl, $Sg(CO)_6$.

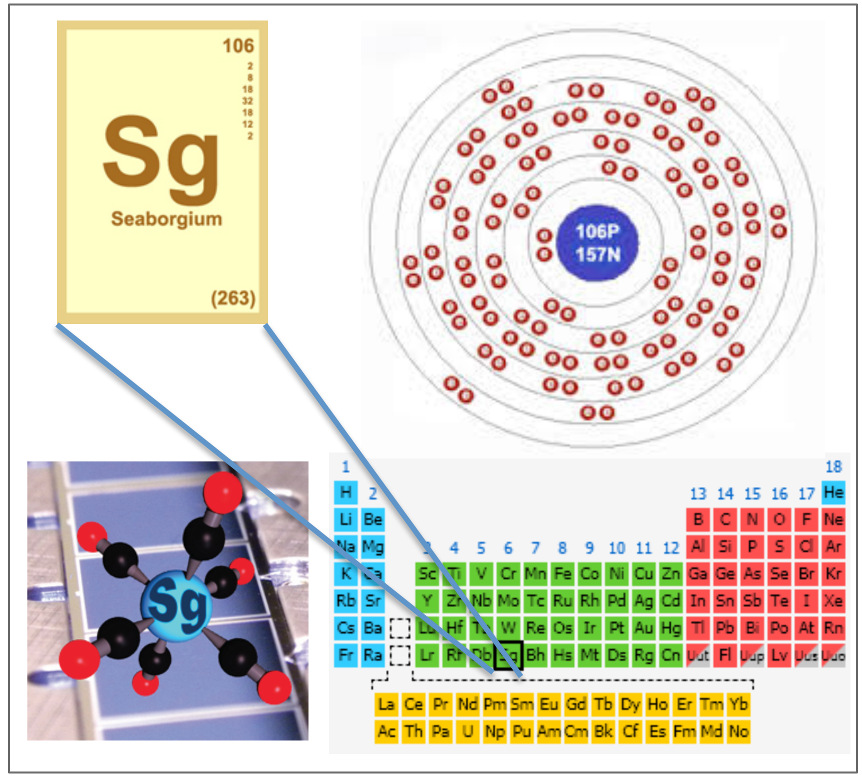
Significance and Impact

Only a few *atoms* of seaborgium can be isolated and they have a half-life of about 2 minutes, so experimental investigations are difficult for this remarkable superheavy element.

Research Details

- All-electron fully relativistic Dirac–Fock and non-relativistic Hartree-Fock SCF calculations.
- First calculations including relativistic effects for the atomization energy, mean bond energy, and energy of the reaction for possible formation of $Sg(CO)_6$
- Acknowledgements in the paper states, "*This supercomputing facility was sine quo non for my massive computations reported herein*."

G. Malli,
The Journal of Chemical Physics 142, 064311 (2015); doi: 10.1063/1.4907595



Element 106 yields to supercomputation: A molecule (lower left) composed of the element seaborgium, which has 106 electrons, has been analyzed using computation that takes into account electronic relativistic effects. A paper published around the same time as this work reports the isolation of the molecule predicted to be stable in NERSC computations.

Work was performed at Simon Fraser U. using NERSC

Electromagnetic Blob Effects in Fusion Plasma

Scientific Achievement

Simulations under conditions relevant to the ITER device have described unwelcome plasma edge effects on filament structures known in the industry as “blobs.”

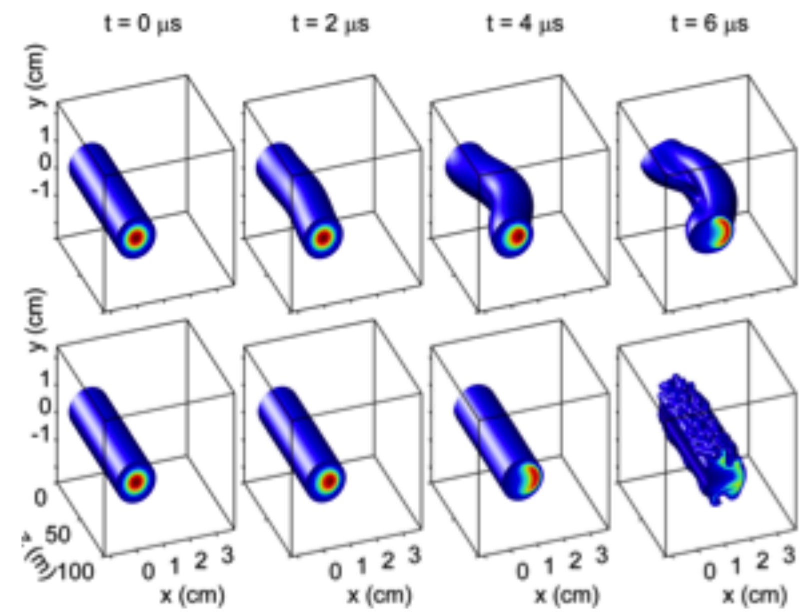
Significance and Impact

Blob turbulence can act like a leak in a tokamak, adversely affecting efficiency and ability to maintain a steady-state plasma.

Research Details

- Simulations show how plasma pressure along the filament leads to of both blob and magnetic field line bending that can can enhance heat exchange between the plasma facing materials and the inner scrape-off layer (SOL) region.
- BOUT++, developed both at LLNL and General Atomics as a finite-difference multi-fluid plasma turbulence code that solves the electromagnetic collisional equations in the complicated geometry near the plasma edge region, was used.

W. Lee, M. Urbansky, and others,
Physics of Plasmas, 22, 012505 (2015); doi: 10.1063/1.4905639

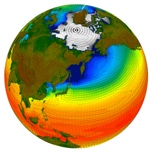


Snapshots comparing electromagnetic and electrostatic simulations using BOUT++ showing evolution of plasma density with time (EM: top; ES: bottom) for a plasma blob, a filamentary structure that extends along magnetic field lines. A typical blob size is 1–3 cm.

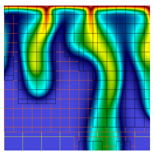
Work was performed at UCSD, LLNL, and NRL using NERSC

About the Title Slide Images

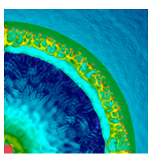
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison; Sponsored by Office of Fusion Energy Sciences



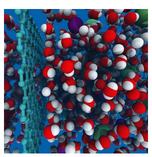
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. Sponsored by Office of Biological and Environmental Research



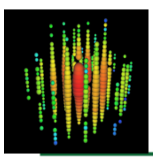
Simulation of density-driven flow for CO_2 storage in saline aquifers. Shown is a snapshot of the CO_2 concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Sponsored by Office of Advanced Scientific Computing Research.



Collision between two shells of matter ejected by a massive star in two pair-instability supernova eruptions, only years apart, just before the star dies, showing a slice through a corner of the event. Shell radius (red knots) is about 500 times the Earth-Sun distance. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Sponsored by Office of High Energy Physics.



Snapshot from a Molecular Dynamics simulation showing water molecules (red and white), and sodium, chloride ions (green and purple) in saltwater, encountering a sheet of graphene (pale blue, center) perforated by holes of the right size, with water passing through (left side), but sodium and chloride being blocked. Provided by D. Cohen-Tanugi and J. C. Grossman, MIT; Sponsored by Office of Basic Energy Sciences



Observation of a PeV-energy neutrino. Each sphere represents a digital optical module sensor in the IceCube detector. Sphere size is a measure of the recorded number of photoelectrons. Colors represent arrival times of photons (red, early; blue, late). Sponsored by Office of Nuclear Physics

National Energy Research Scientific Computing Center