NERSC Science Highlights

A selection of recent results

June 2012
Scientific Accomplishments at NERSC

**Analytics**
Parallel I/O on Hopper plus new hybrid-parallel query techniques support analysis of trillion-particle plasma simulation
(S. Byna, LBNL)

**Chemistry**
Multiscale molecular simulations provide important insight into a molecule that can mimic photosynthesis
(M. Cheung, U. Houston)

**Fusion**
NDCX-II simulations help clear the path to heavy ion fusion power
(A. Friedman, LBNL)

**Materials**
Molecular simulations demonstrate how to tune nanoporous graphene for gas separations
(J. Schrier, Haverford)

**Energy**
NERSC simulations suggest promise for supercapacitor energy based on a class of materials called onion carbons
(D. Jiang, ORNL)

**High Energy Physics**
GEANT4 and other simulations on Hopper are helping to unlock mysteries of the neutrino
(G. Gratta, Stanford)
• Onion-like carbons (OLCs) consist of concentric layers of graphene sheets.

• Can be used in a novel class of energy storage devices called supercapacitors.

• Excellent durability and higher power density, capacitance, and charging/discharging rates than conventional capacitors.

• Molecular Dynamics has, for the first time, explained the relationship between capacitance and electrode potential in these supercapacitors.
  
  • Especially the Influence of electrode curvature and size
  
  • Work done for DOE’s “Fluid Interface Reactions, Structures, and Transport” (FIRST) Center, an EFRC

PIs: D. Jiang (ORNL); P. Cummings (Vanderbilt)
• Margaret Cheung and coworkers performed multiscale molecular simulations to explore the role that confinement, temperature, and solvents play in the stability and energy efficiency of a light-harvesting triad, a novel material that converts sunlight into chemical energy by mimicking photosynthesis.

• Results could provide a way to test, tailor, and engineer molecules that, when combined in large numbers, could greatly increase the ability to produce clean energy.
First-ever *trillion-particle* plasma physics simulation conducted on 120,000 Hopper cores to study magnetic reconnection phenomena.

- Achieved 35 GB/s sustained I/O rate (80% of peak).
- FastBit was used to index 30 TB of data in 10 minutes and query in 3 seconds.
- Software enabled scientists to examine and gain insights from the trillion particle dataset for the first time:
  - Confinement of energetic particles by the flux ropes.
  - Asymmetric distribution of particles near the reconnection hot-spot.

Magnetic reconnection from a plasma physics simulation (Left). Scientists were able to query and find an asymmetric distribution of particles near the reconnection event (Right) using our software tools.

**Pls:** Prabhat, S. Byna (LBNL); H. Karimabadi (UCSD)
• GEANT4 and other simulations on Hopper have validated the most sensitive measurements ever in a decades-long hunt for a hypothetical and rare decay process involving particles that are their own antiparticle.
  – The measurements have resulted in non-detection, which has set a lower bound on the half-life of neutrino-less double-beta decay.
  – Has also narrowed down the range of possible masses for the neutrino

• More recent work is including electric field effects to improve simulation of the detector response

Two kinds of double-beta decay, in which two neutrons transmute into two protons, either with neutrino emission (left) or neutrinoless (right), where neutrinos are their own antiparticles and they self-annihilate.

The EXO-200 apparatus that is attempting to search for neutrinoless double beta decay in a large volume of highly-enriched $^{136}$Xe

Unlocking Mysteries of the Neutrino
– Goal: Evaluate the feasibility of separating gas mixtures using nanoporous graphene “filters”

– Application to CO$_2$ sequestration, biogas upgrading, SO$_2$ pollution control, air dehumidification

– Molecular simulations demonstrate how to tune filter selectivity for the different gases and applications.

– Large number of NERSC molecular dynamics simulations required to cover all species and conditions.

NERSC “NISE” Project
NERSC ATG staff recently *tripled* performance by optimizing the domain decomposition.

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PI: J. Schrier (Haverford)
• The LBNL Neutralized Drift Compression Experiment (NDCX-II) is an accelerator used to study how to produce compact, intense, short-pulse ion beams for heavy-ion fusion.

• The system was designed in part using many simulations run at NERSC.
  – Used the Warp3D code, which combines Particle-In-Cell with accelerator effects
  – Hundreds of parallel runs used to set and design tolerances for various accelerator elements and to tune accelerator solenoids
  – NERSC staff research improved Python & shared-library performance for Warp3D; speedups of 4-10X
• Simulating Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) at NERSC allows
  – first-principles interpretation of ALS data, leading to deeper understanding of basic chemical structure and reactivity
  – promotion of closer interaction between theory and experiment
  – more efficient and complete use of DOE synchrotron light source facility

• Accomplishment: Electronic structure of aqueous boron-hydride complexes (which are considered as good prospects for transportable hydrogen storage materials) yields understanding of how hydrogen is actually produced (PCCP cover story)

• Accomplishment: New and detailed insights into the nature of CO$_2$ dissolution in water – a fundamental process governing the terrestrial carbon cycle (Chemical Physics Letters “Frontiers” article)
The chemical reaction of NO$_2$ with a zeolite catalyst was studied via density functional theory.

- Important because of the need to reduce emissions of NO$_x$ from automobiles and the potential use of zeolite catalysts for this purpose.
- The study identified atomic level aspects of the reaction mechanism not available from experiments.
- Results provide fundamental information about how these kinds of catalysts work.
Magnetic Instabilities in NSTX and ITER

- Magnetohydrodynamic plasma simulations have reproduced the experimental observation of magnetic island instabilities that saturate and persist in the National Spherical Torus eXperiment (NSTX).
  - These “tearing modes” have no apparent triggering event but can lead the plasma to disrupt.
- Nonlinear magnetohydrodynamic studies are essential for developing a predictive model for tokamaks such as ITER.
  - The predictive capability demonstrated in this work provides some confidence of predicting the onset of these modes in ITER, should they exist.

(a) Cross-section of the NSTX tokomak. (b) Top: Measured NSTX shot data. Bottom: Simulated plasma without (left) and with (right) instability.

Contours of the perturbed toroidal current density, pressure, vorticity, compressible velocity potential, and toroidal velocity computed by the M3D code.

PI: S. Jardin (PPPL)