NERSC Science Highlights

A selection of recent results

June 2012

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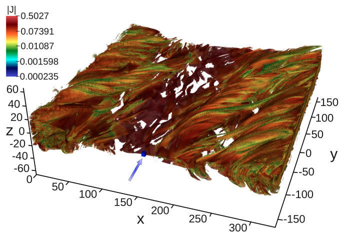
NERSC National Energy Research Scientific Computing Center

BERKELEY LAB Lawrence Berkeley National Laboratory

Scientific Accomplishments at NERSC



Analytics

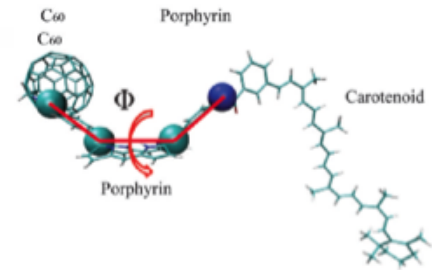
Parallel I/O on Hopper plus new hybrid-parallel query techniques support analysis of trillion-particle plasma simulation

(S. Byna, LBNL)

Chemistry

Multiscale molecular simulations provide important insight into a molecule that can mimic photosynthesis

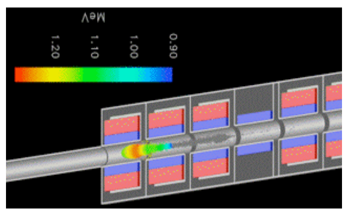
(M. Cheung, U. Houston)

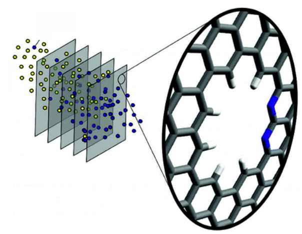


Fusion

NDCX-II simulations help clear the path to heavy ion fusion power

(A. Friedman, LBNL)

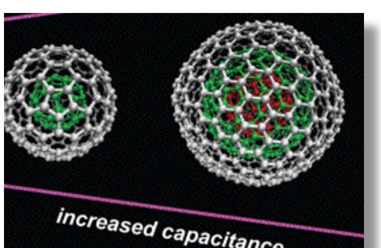




Materials

Molecular simulations demonstrate how to tune nanoporous graphene for gas separations

(J. Schrier, Haverford)



Energy

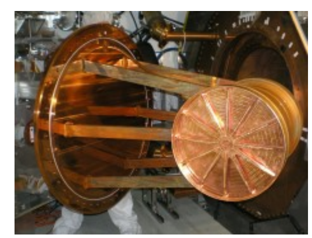
NERSC simulations suggest promise for supercapcitor energy based on a class of materials called onion carbons

(D. Jiang, ORNL)

High Energy Physics

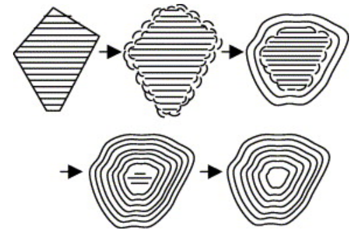
GEANT4 and other simulations on Hopper are helping to unlock mysteries of the neutrino

(G. Gratta, Stanford)

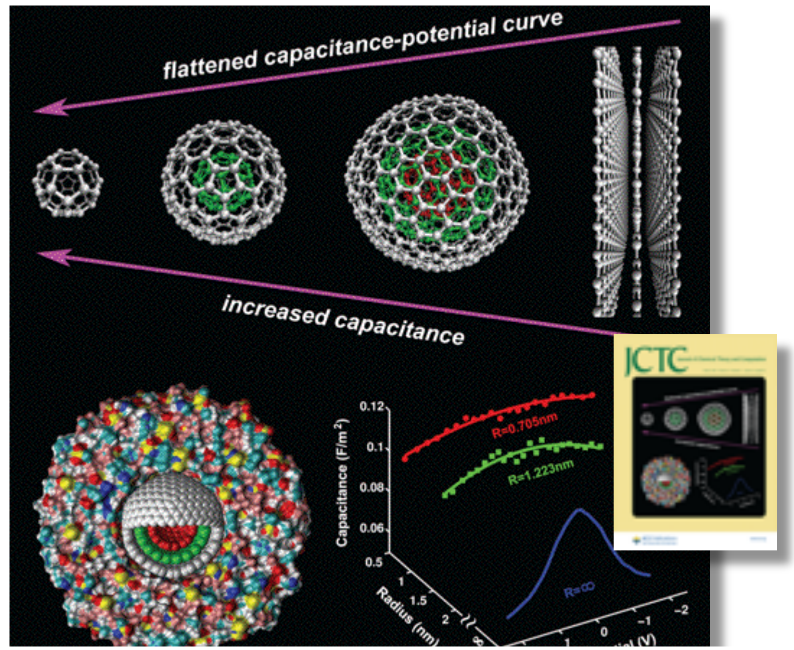


Promise for Onion-Like Carbons as Supercapacitors

- **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**



How graphene becomes onion-like.



Some of the capacitance / geometry effects revealed by molecular dynamics simulations at NERSC and reported as the cover story of the Journal of Chemical Theory and Computation, March 13 2012.

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BES

PIs: D. Jiang (ORNL); P. Cummings (Vanderbilt)

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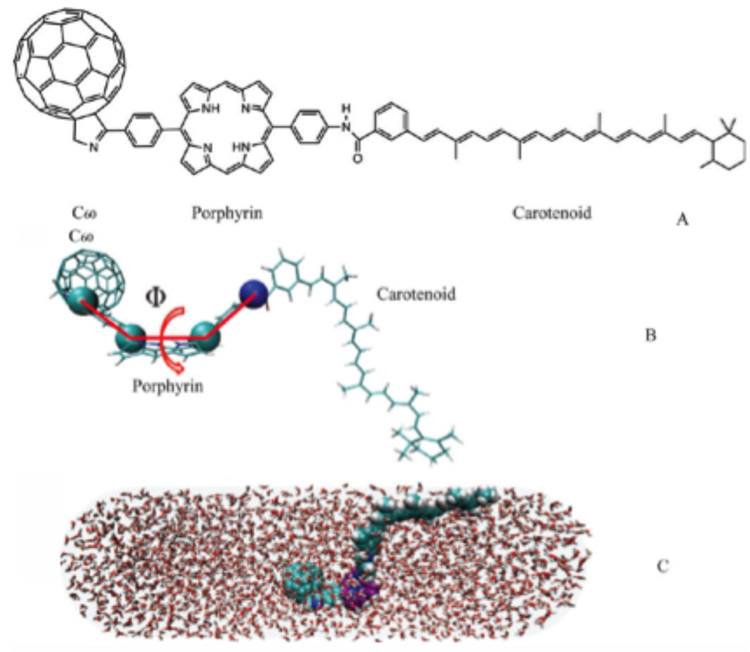
Learning from Photosynthesis

- **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.**



Three views of the molecule that imitates photosynthesis. Top: chemical formula; middle: 3-D structure; bottom: A snapshot of an all-atomistic simulation of the molecule in water done at NERSC

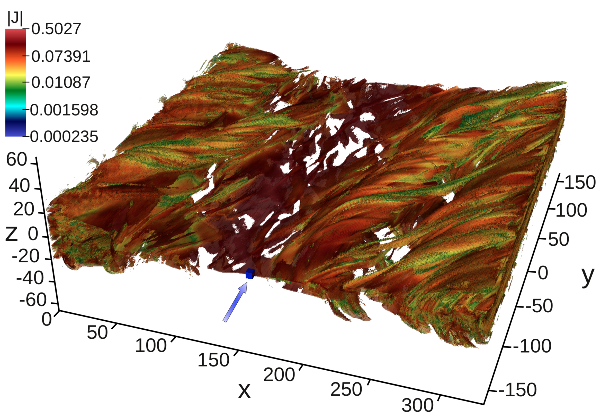
THE JOURNAL OF PHYSICAL CHEMISTRY B DOI: 10.1021/jp212273n

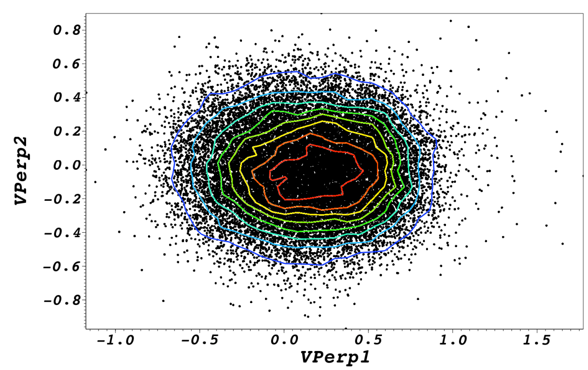
BES

PIs: M. Cheung (U. Houston)

Science at Scale: Parallel I/O Supports Analysis of Trillion-Particle Simulation

- 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.

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ASCR
PIs: Prabhat, S. Byna (LBNL); H. Karimabadi (UCSD)
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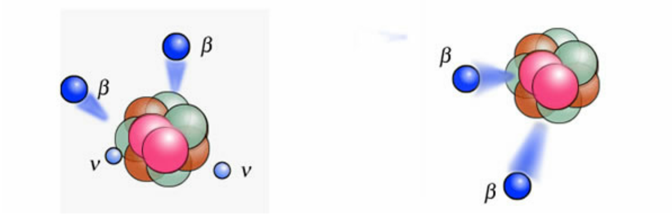
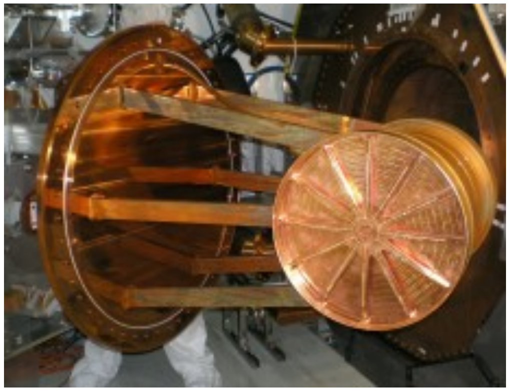
Unlocking Mysteries of the Neutrino

- **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-anhilate.



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

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HEP

PI: G. Gratta (Stanford); M. Marino (Tech U Munich)

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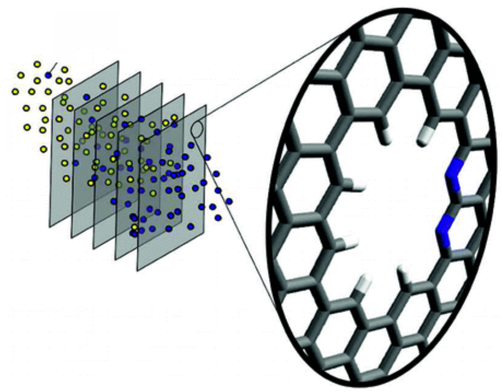
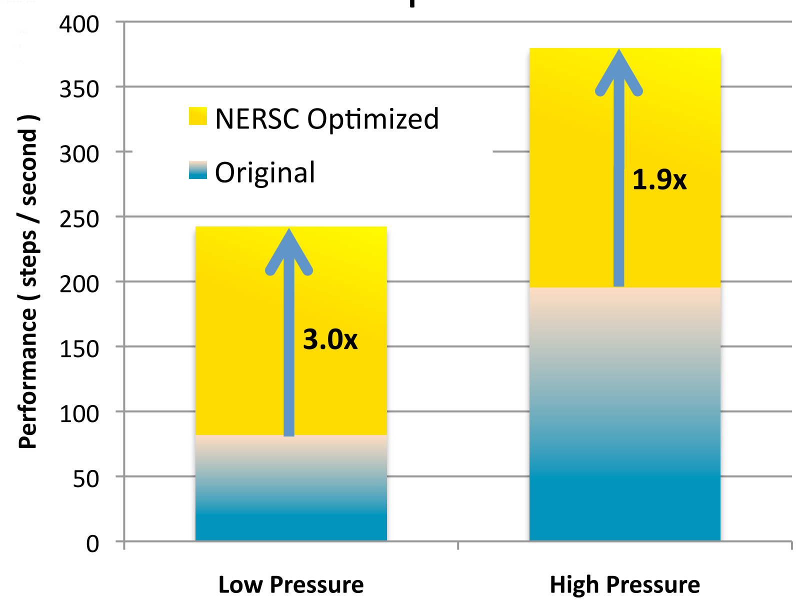
Tuning Nanoporous Graphene for Gas Separation

- 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.



ACS APPLIED MATERIALS & INTERFACES 2011, 3, 4451–4458

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BES

PI: J. Schrier (Haverford)

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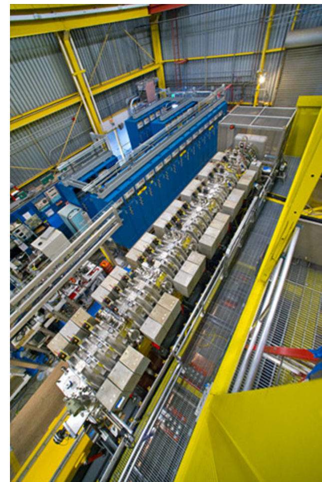
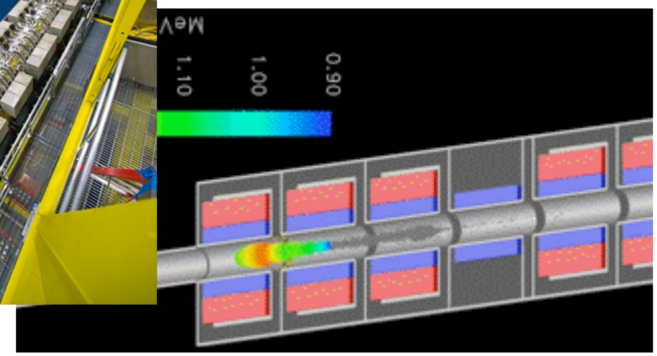
Science Through Volume: NDCX-II Simulations Help Clear the Path to Heavy Ion Fusion Power

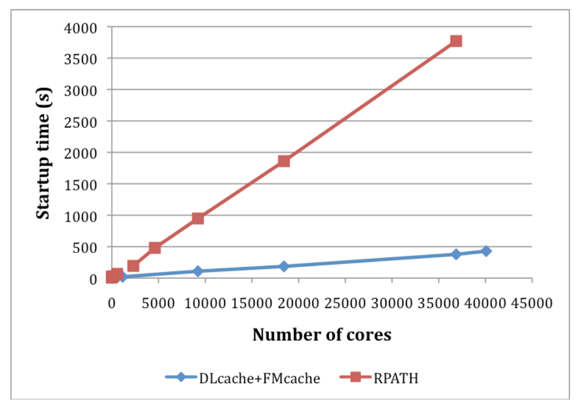
- **The LBNL Neutralized Drift Compression Experiment (NDCX-II) is an accelerator used to study how to produce compact, intense, short-pulse ion beams for heavy-ion fusion.**
- **The system was designed in part using many simulations run at NERSC.**
  - Used the Warp3D code, which combines Particle-In-Cell 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



The real NDCX-II system.



Portion of a 12-cell NDCX-II Warp3D simulation showing a beam bunch exiting to the left.



Warp3D startup times on Hopper (red=original, blue=improved) from Cray User Group paper by Cray and NERSC staff

FES

PIs: A. Friedman, D. Grote (LBNL)

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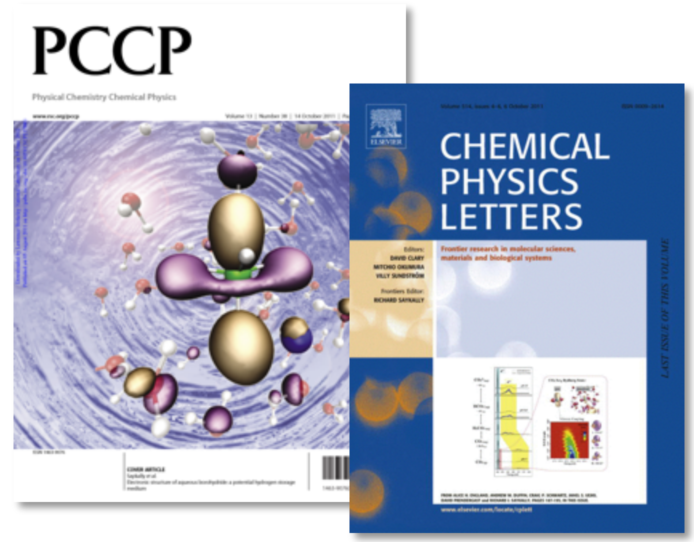
Science and Energy Insight from NERSC + ALS

- **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)**



Prendergast and Saykally, PIs

- **Accomplishment: New and detailed insights into the nature of CO_2 dissolution in water – a fundemental process governing the terrestrial carbon cycle (Chemical Physics Letters "Frontiers" article)**

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PIs: R. Saykally (UC Berkeley); D. Prendergast (LBNL)

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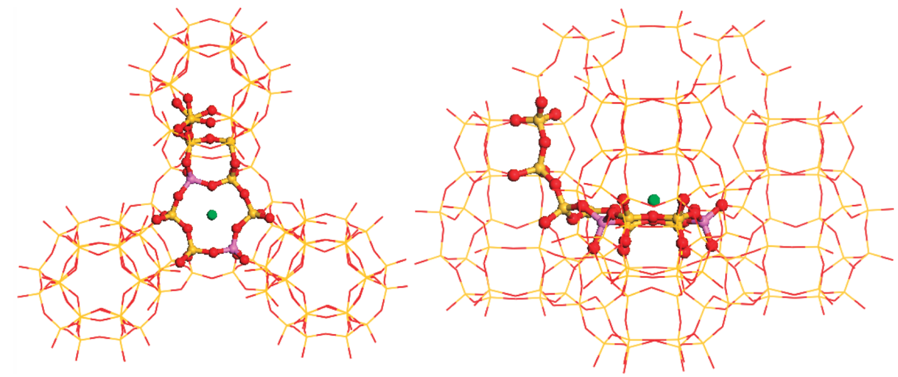
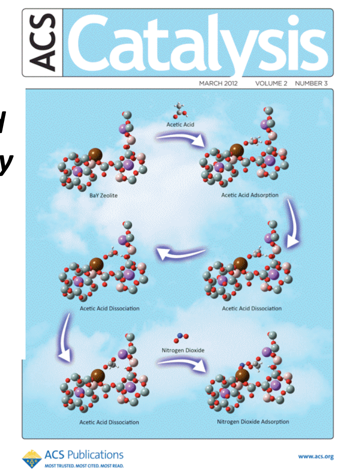
Computations Reveal Mechanism of Catalytic Reduction of Nitrogen Dioxide

- **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.





Two views of the zeolite studied (top) and artwork from the study appearing on the cover of the American Chemical Society Journal "Catalysis, January 30, 2012"

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PIs: L. Broadbelt, R. Snurr (Northwestern

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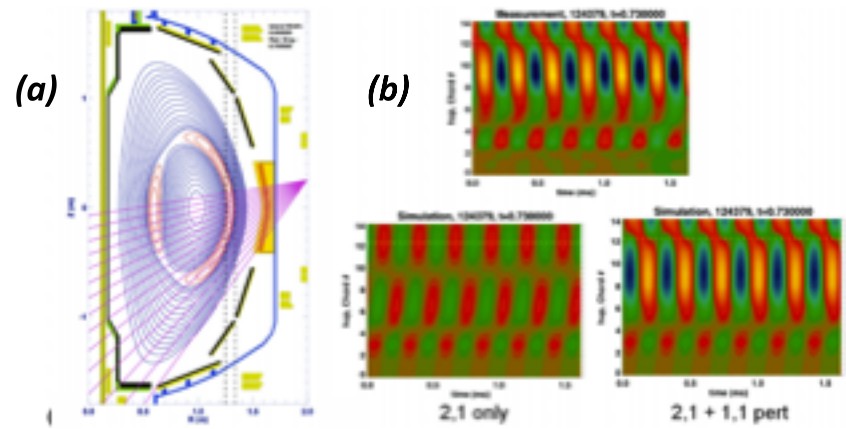
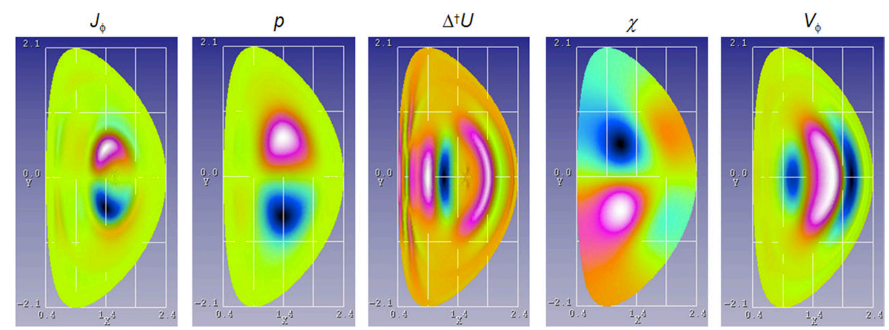
Magnetic Instabilities in NSTX and ITER

- **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 tokamak.
(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.

FES

PI: S. Jardin (PPPL)