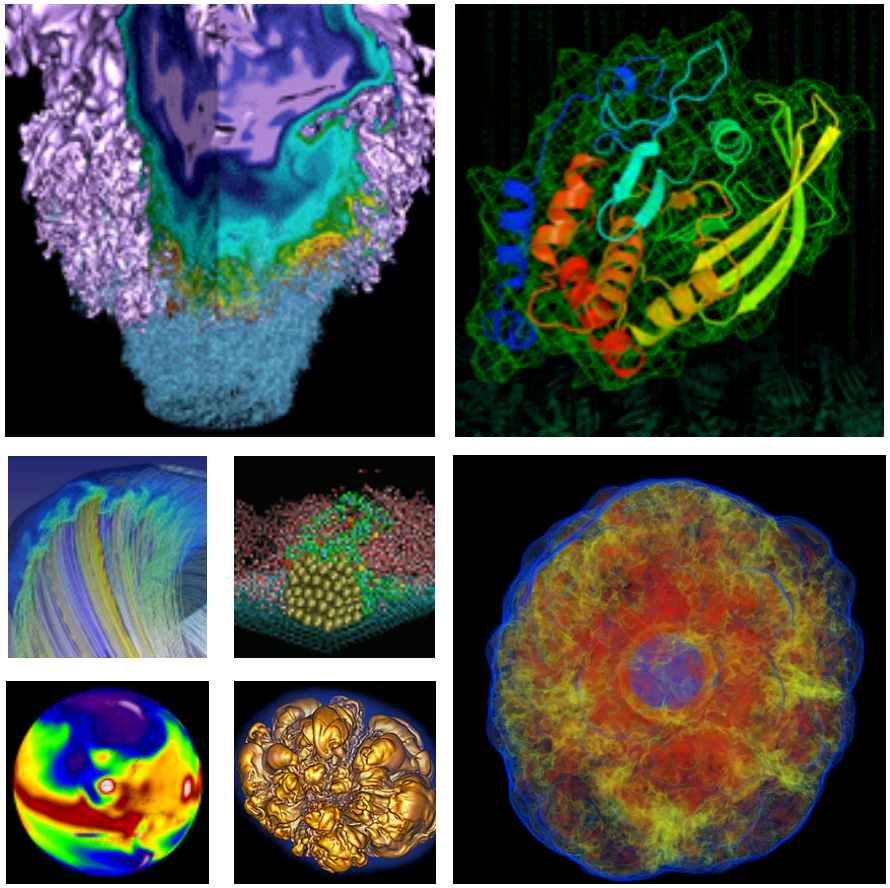
NERSC Overview



David Turner
NERSC User Services Group

NERSC 40 YEARS at the FOREFRONT 1974-2014

NUG New User Training
February 23, 2015

U.S. DEPARTMENT OF ENERGY | Office of Science

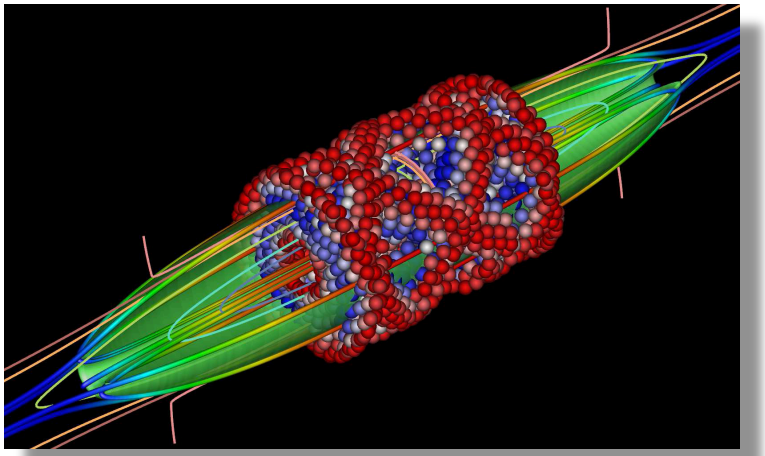
BERKELEY LAB Lawrence Berkeley National Laboratory

NERSC

- **National Energy Research Scientific Computing Center**
  - Established 1974, first unclassified supercomputer center
  - Original mission: to enable computational science as a complement to magnetically controlled plasma experiment
- Today's mission: ***Accelerate scientific discovery at the DOE Office of Science through high performance computing and extreme data analysis***
- A national user facility

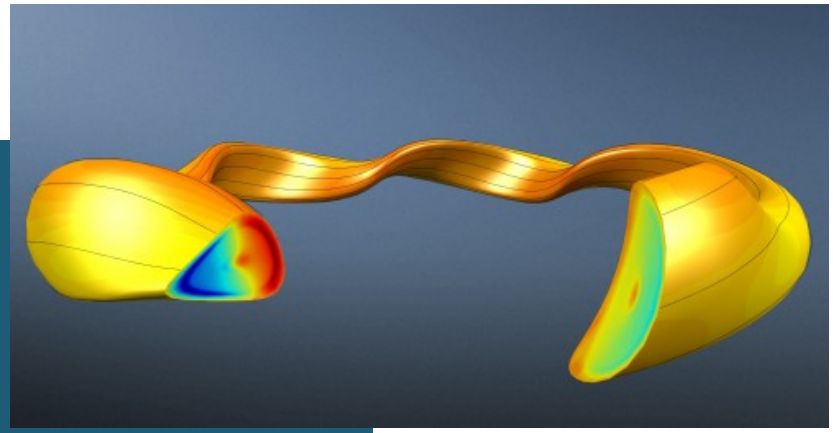
Today's Talk

- **A brief introduction to the Center and some simple rules for getting work done at NERSC.**



Trajectory of an energetic ion in a Field Reverse Configuration (FRC) magnetic field. Magnetic separatrix denoted by green surface. Spheres are colored by azimuthal velocity. Image courtesy of Charlson Kim, U. of Washington; NERSC repos m487, mp21, m1552

You Are Not Alone !



A calculation of the self-generated plasma current in the W7-X reactor, performed using the SFINCS code on Edison. The colors represent the amount of electric current along the magnetic field, and the black lines show magnetic field lines. Image: Matt Landreman

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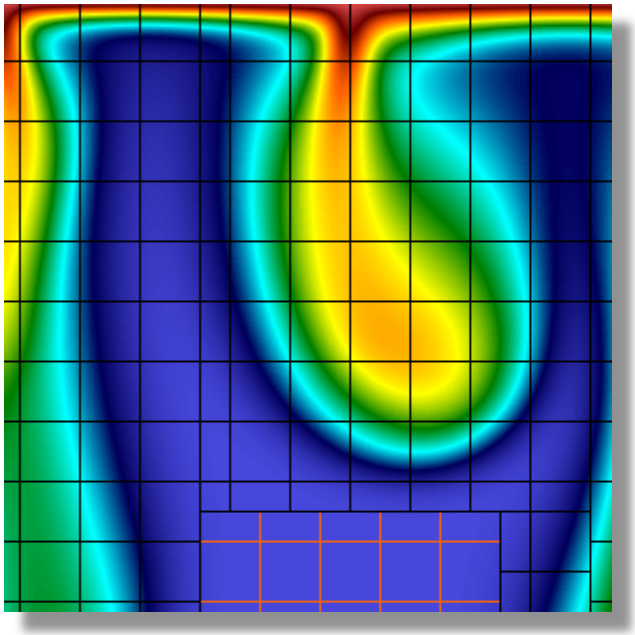
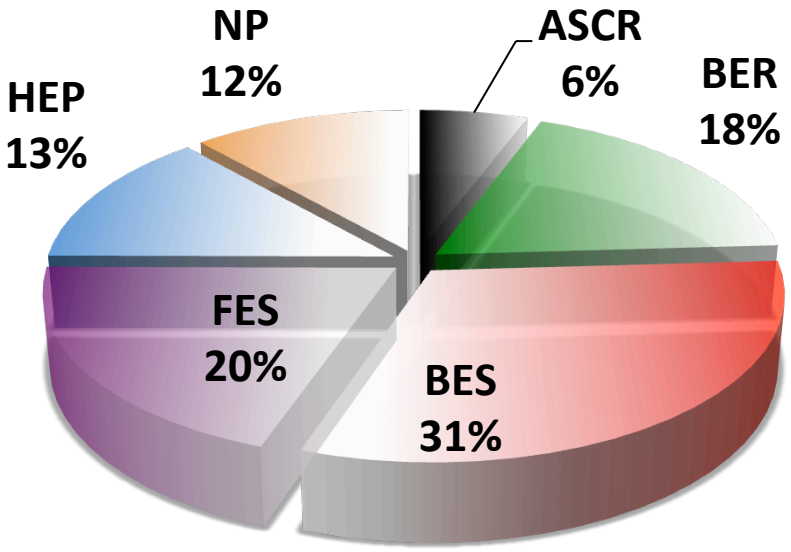
NERSC: Mission Science Computing for the DOE Office of Science

- **Diverse workload:**
  - 4,500 users, 700+ projects
  - 700 codes; 100s of users daily
- **Allocations controlled primarily by DOE**
  - 80% DOE Annual Production awards (ERCAP):
    - From 10K hour to ~10M hour
    - Proposal-based; DOE chooses
  - 10% DOE ASCR Leadership Computing Challenge
  - 10% NERSC reserve
    - NISE, NESAP



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). Repo mp111

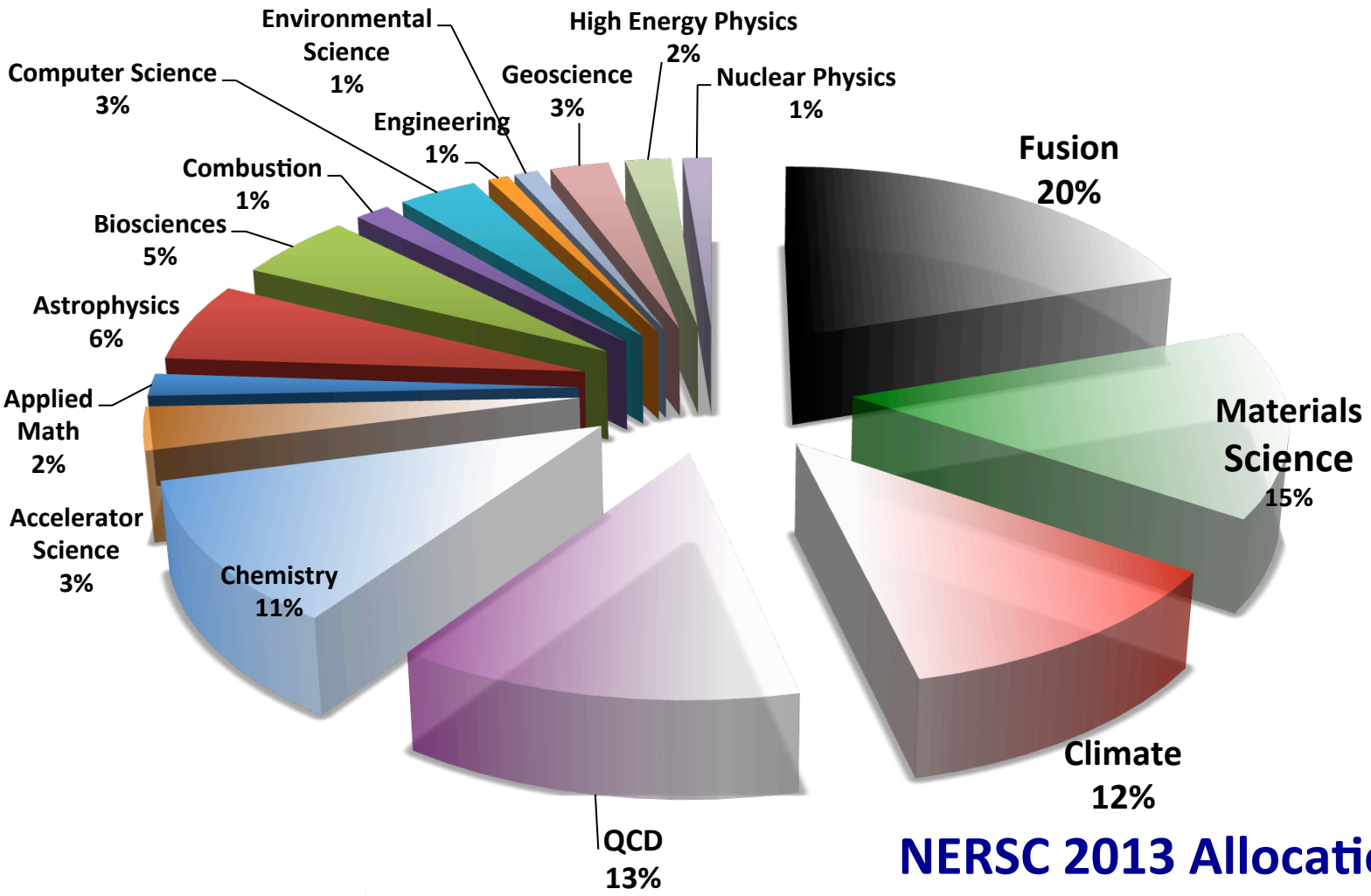
DOE View of Workload



NERSC 2013 Allocations By DOE Office

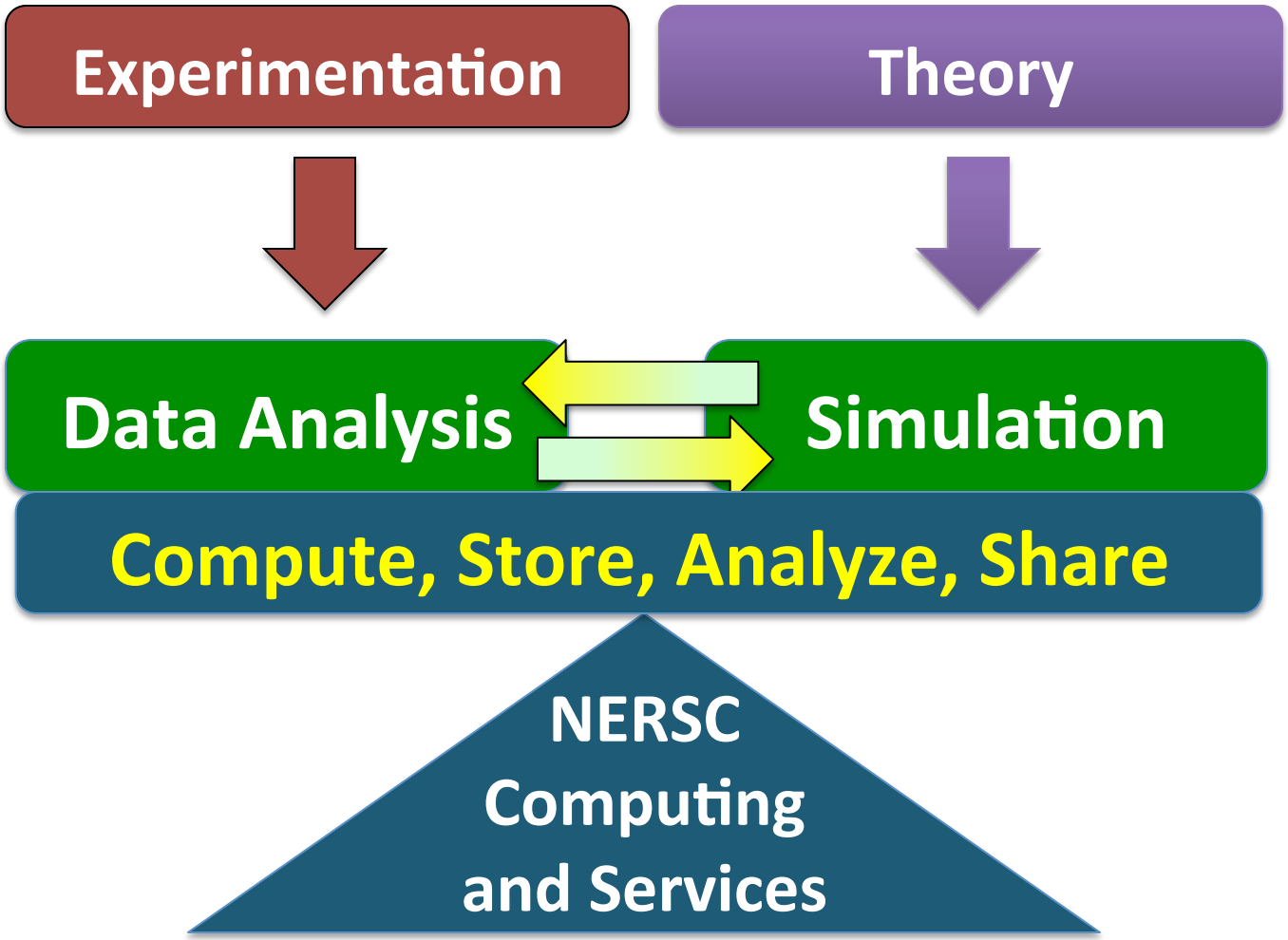
ASCR	Advanced Scientific Computing Research
BER	Biological & Environmental Research
BES	Basic Energy Sciences
FES	Fusion Energy Sciences
HEP	High Energy Physics
NP	Nuclear Physics

Science View of Workload

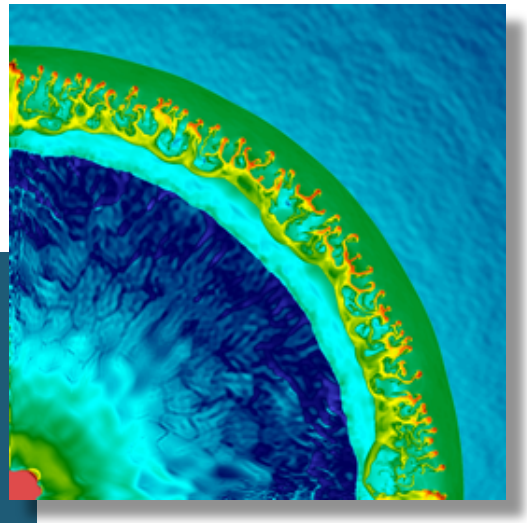


NERSC 2013 Allocations By Science Area

What Role Does NERSC Play?



You Will Be Successful !



Collision between two shells of matter ejected in two supernova eruptions, showing a slice through a corner of the event. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Repo m1400

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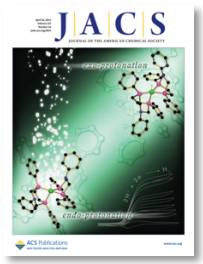
Journal Cover Stories from NERSC-Enabled Research 2013

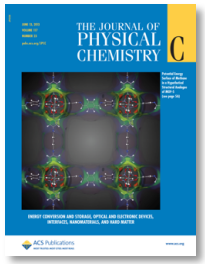
Leung, Sandia
BES

Wu, ColoMines
BES

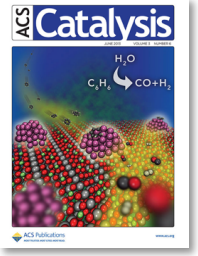


Raugei, PNNL
BES

Striolo, Oklahoma
BES



Smit, LBNL
BES



Mei, PNNL
BES

Compo, Colorado
BER

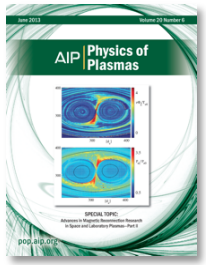
Persson, LBNL
BES

Ha, LBNL
NP

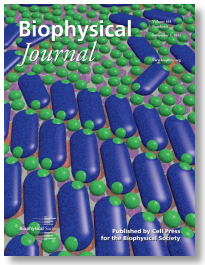
Whitelam, LBNL
BES

Daggett, Washington
BER

Mei, PNNL
BES

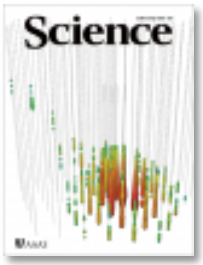


Daughton, LANL
FES

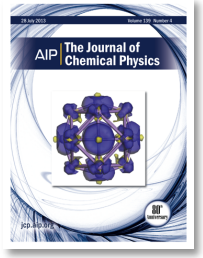


Geissler, UC B
BES

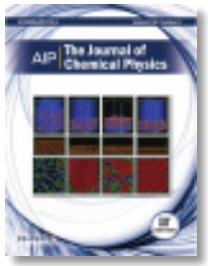
Ghattyvenkatakrishna, FSU
BER



Ha, LBNL
NP



Jena, VCU
BES



Grest, Sandia
BES

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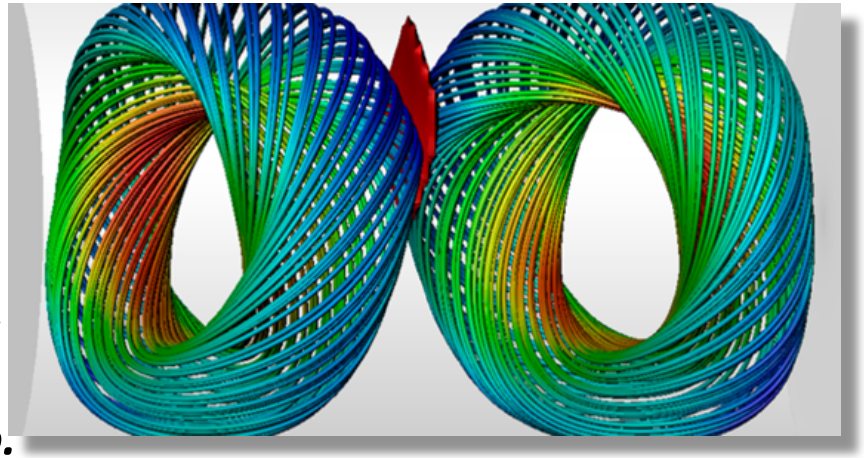
NERSC Users Report ~1,500 Publications / Year

- **Make sure you acknowledge NERSC in publications; please use "official" acknowledgement**
- **https://www.nersc.gov/users/accounts/user-accounts/acknowledge-nersc/**

- ***This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.***

- **Science highlights sent to DOE each quarter.**
  - Send us links to your publications.



Magnetic field lines from HiFi simulations of two spheromaks. NERSC repo m1255 Image courtesy of Vyacheslav Lukin (NRL)

NERSC Systems Today

System Choices

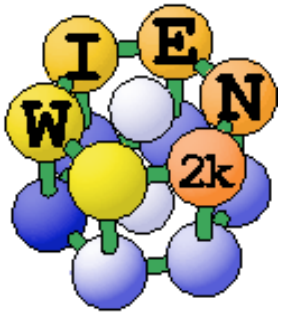
- **Edison: fastest processors; fastest interconnect; best for scaling to large core counts; higher NERSC machine charging factor**
- **Hopper: previous generation processors; excellent scalability; lower charge factor**
- **Carver: compute nodes have more generic linux; current serial queue**

Simple Rules for Success

- Use our web site; use “Search…”
- Cray systems are not “typical” clusters, pay attention to differences
- Be kind to your neighbor users
- Back your stuff up
- Pick the right resource for your job and your data
- Use batch system effectively; pay attention to system-specific syntax and policies
- Use your allocation smartly
- Pay attention to security

Chemistry & Materials Applications

- **NERSC compiles and supports many software packages for our users.**



BerkeleyGW

QUANTUMESPRESSO

Molpro

LAMMPS

abinit.

siesta

NAMD

Scalable Molecular Dynamics

- *More than 13.5 million lines of source code Compiled, Optimized, and Tested*

b-initio

VASP

ackage

imulation

lenna

GAMESS

Q-CHEM

GAUSSIAN

WANNIER90

CPMD

NWCHEM

HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

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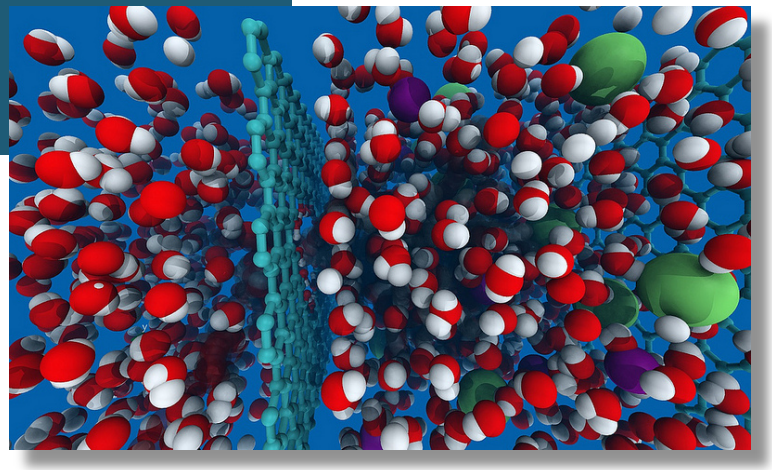
NERSC User's Group

- Get involved. Make NUG work for you.
- Provide advice, feedback – we listen.
- Monthly teleconferences with NERSC, usually the last Thursday of the month, 11:00 AM to noon Pacific Time.
- Executive Committee - three representatives from each office and three members-at-large.
- Community!

Rule # 4: Expect Consistency. And Change.



Molecular Dynamics simulation snapshot showing water molecules (red and white), and sodium, chloride ions (green and purple) 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.

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NERSC Roadmap

Peak Teraflop/s

10^7
10^6
10^5
10^4
10^3
10^2
10

N10 ~1 EF Peak
N9 200-500 PF Peak
Cori (N8) 10-30x Hopper
Edison (N7)
2.4 PF Peak
Hopper (N6)
1.25 PF Peak
Franklin (N5) +QC
36 TF Sustained
352 TF Peak

2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

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Change and Consistency

- **NERSC will be physically moving to a new facility in 2015.**
- **Carver will retire September 30, 2015.**
- **Hopper will retire December, 2015.**
- **NERSC-8 (Cori)**
  - Phase 1 Haswell late summer 2015
  - Phase 2 Knights Landing summer 2016
  - **Disruptive change**
    - Codes likely will run, but will need to be modified to achieve good performance
  - NERSC will help users make this transition.
- **Edison will remain available for codes that cannot transition to NERSC-8**

Thank you and welcome to NERSC!

Generic Multiprocessor Architecture