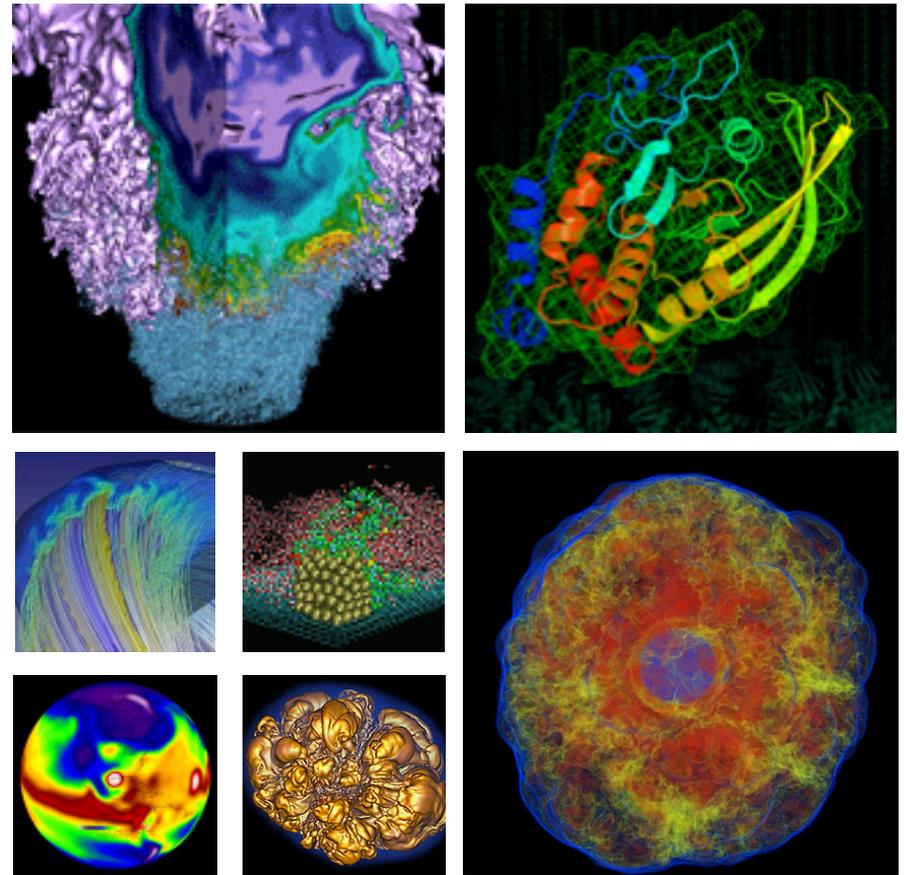


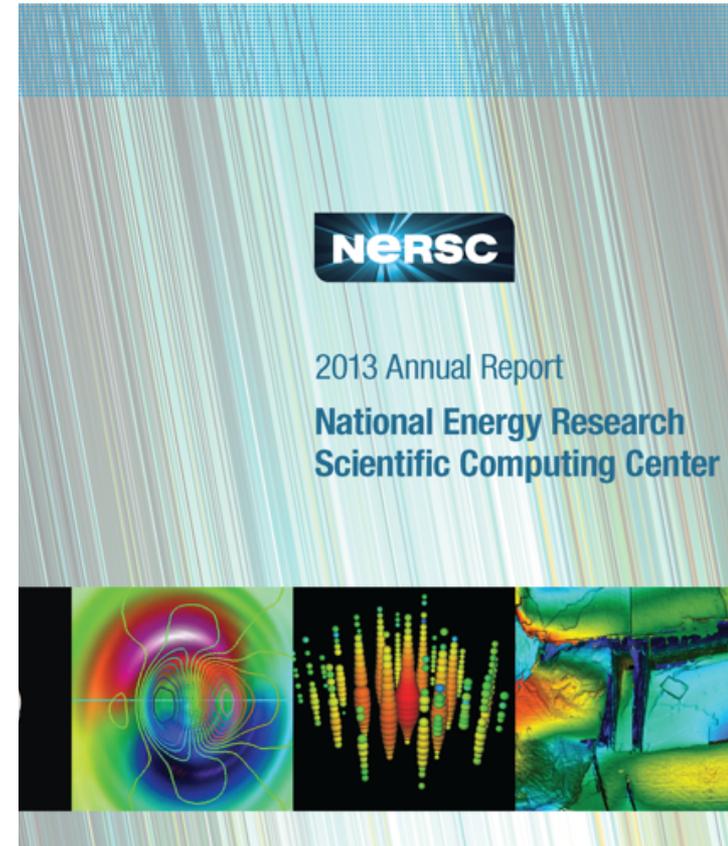
# NERSC Overview



**David Turner**  
**NERSC User Services Group**

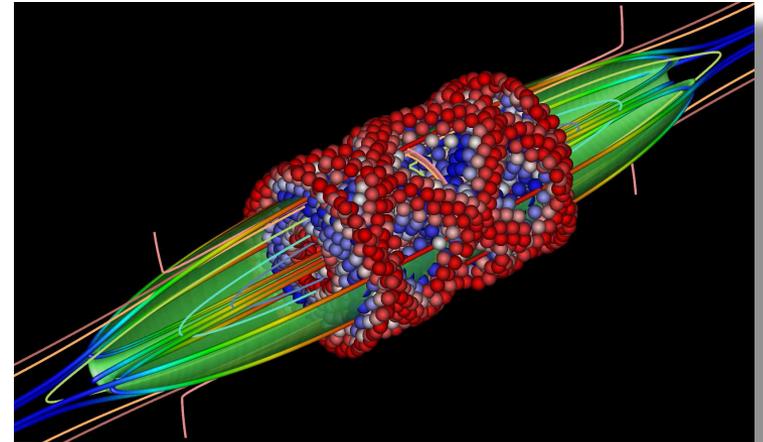
**New User Training**  
**October 30, 2014**

- **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



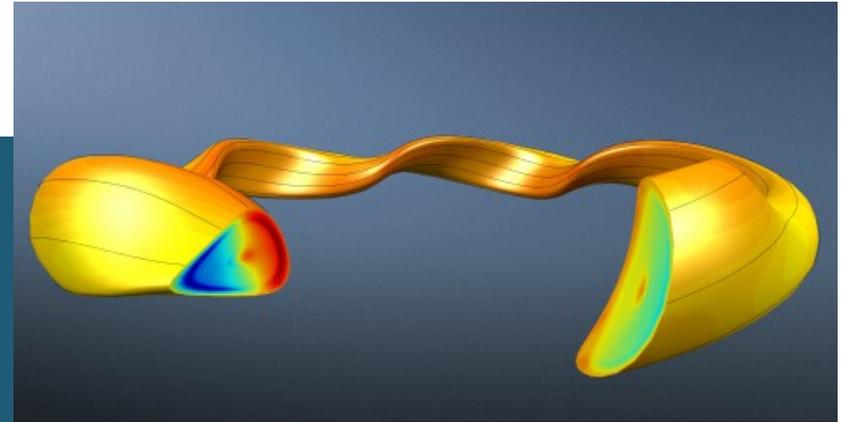
# Today's Talk

- 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*

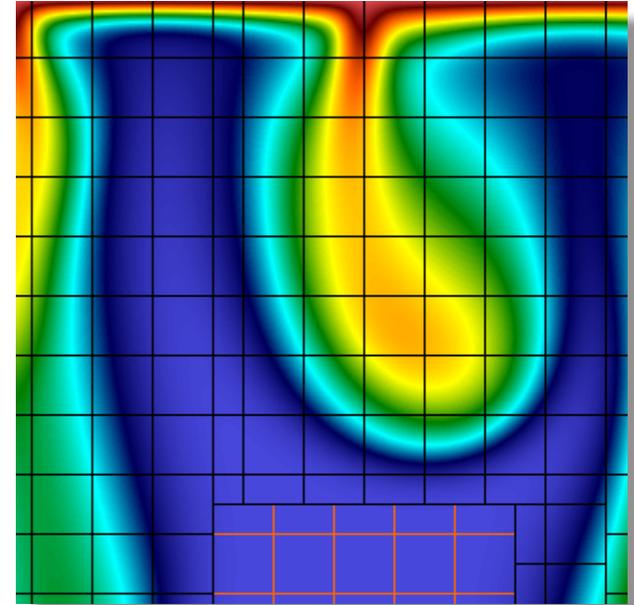
# You Are Not Alone !



*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*

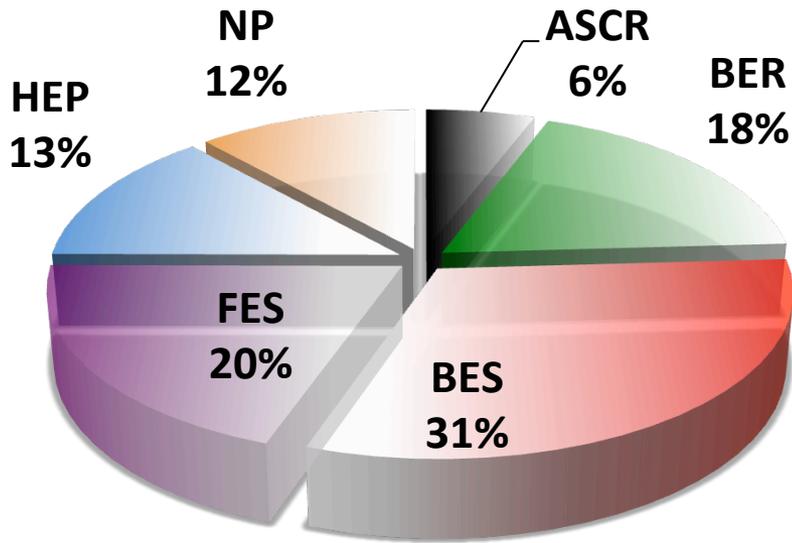


- **Diverse workload:**
  - 4,500 users, 700+ projects
  - 700 codes; 100s of users daily
- **Allocations controlled primarily by DOE**
  - 80% DOE Annual Production awards (ERCAP):
    - From 10K hour to ~10M hour
    - Proposal-based; DOE chooses
  - 10% DOE ASCR Leadership Computing Challenge
  -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



*Simulation of density-driven flow for CO<sub>2</sub> storage in saline aquifers. Shown is a snapshot of the CO<sub>2</sub> concentration after onset of convection overlaid 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**

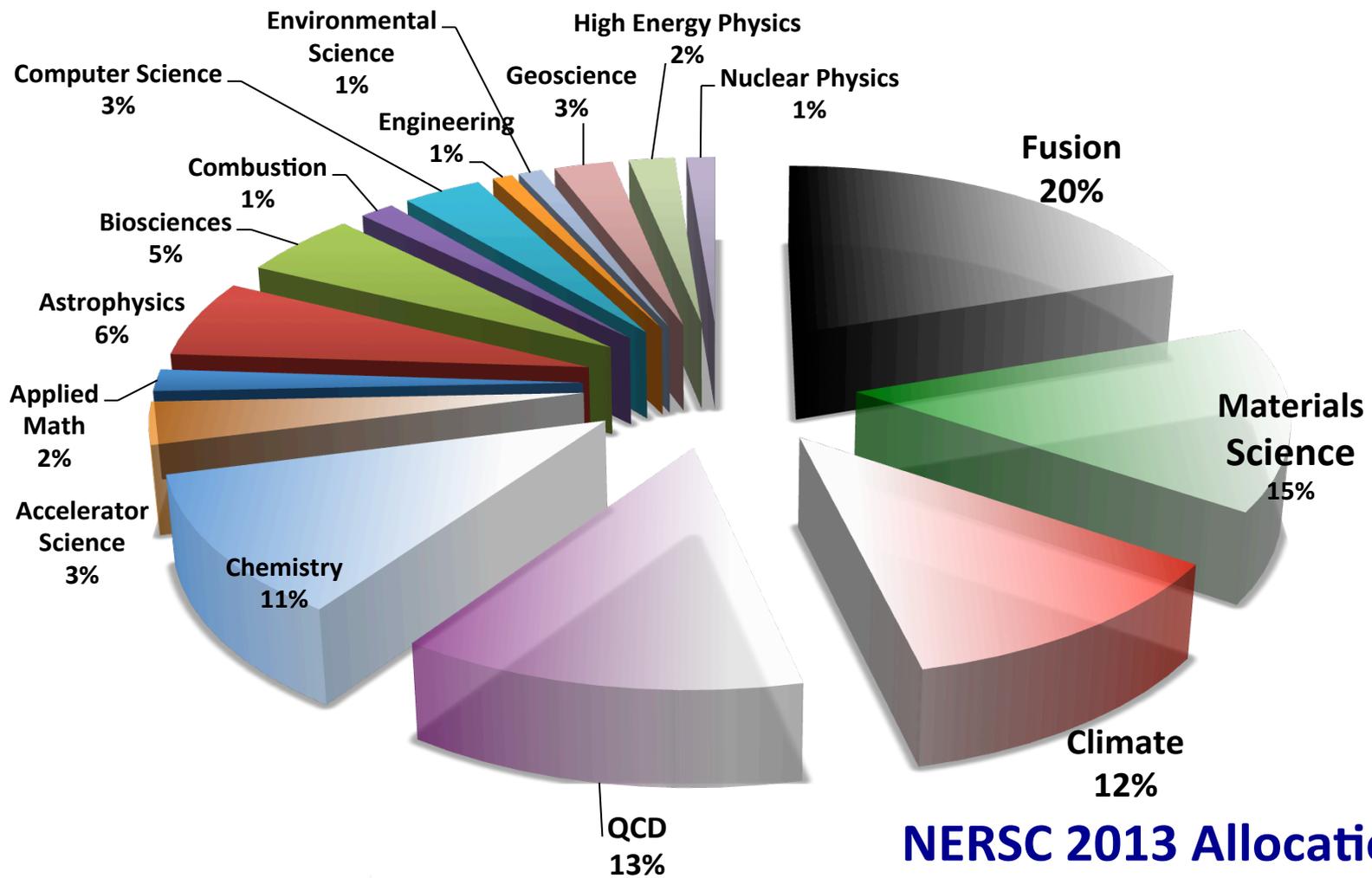
**BES**      **Basic Energy Sciences**

**FES**      **Fusion Energy Sciences**

**HEP**      **High Energy Physics**

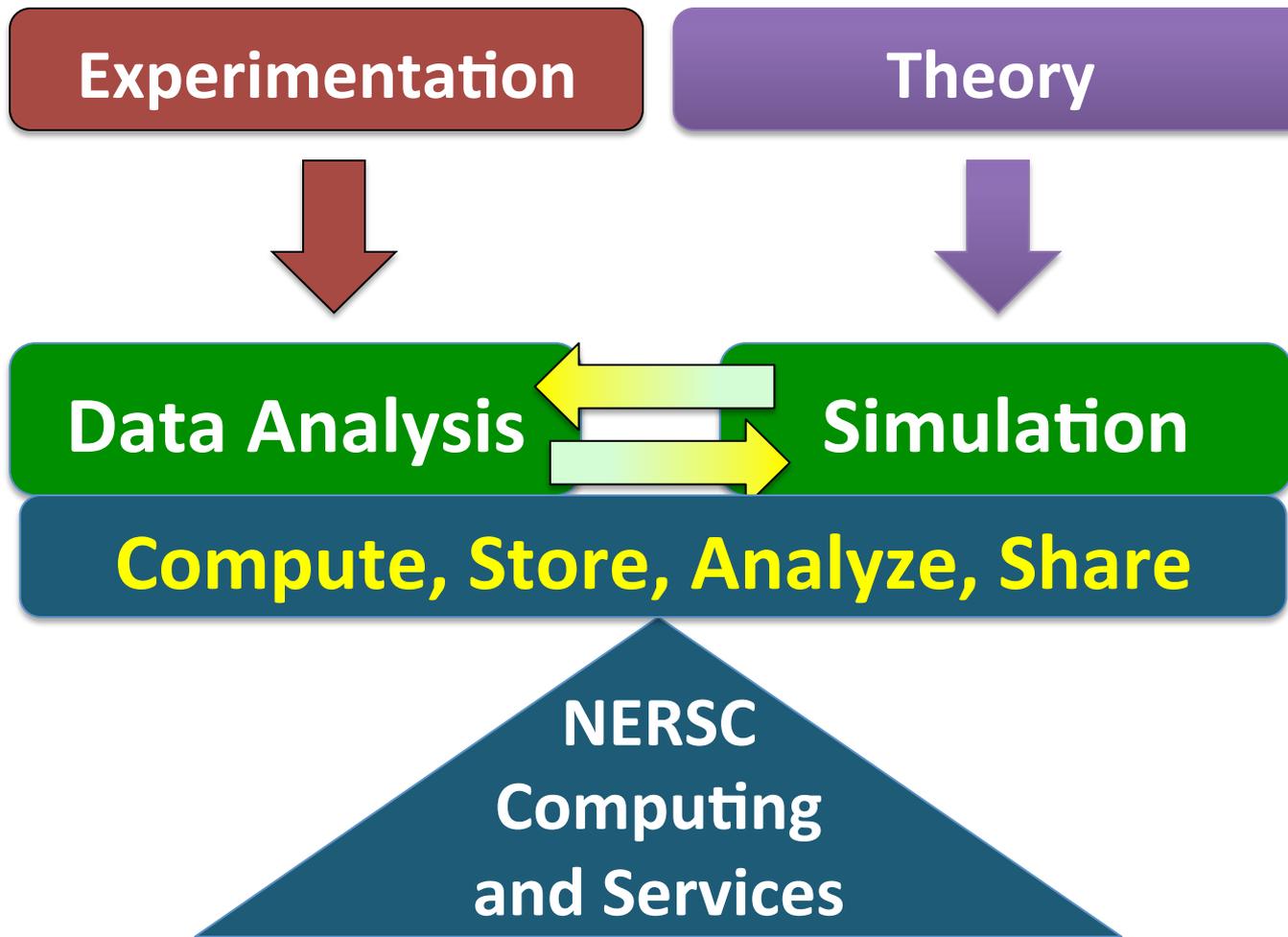
**NP**      **Nuclear Physics**

# Science View of Workload

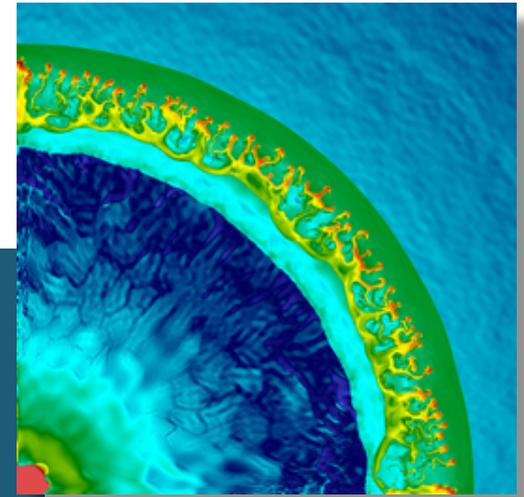


**NERSC 2013 Allocations  
By Science Area**

# What Role Does NERSC Play?



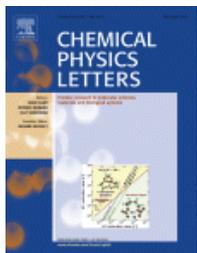
# You Will Be Successful !



*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*



# Journal Cover Stories from NERSC-Enabled Research 2013



Leung, Sandia  
BES



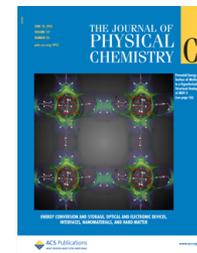
Wu, ColoMines  
BES



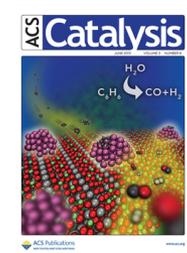
Raugei, PNNL  
BES



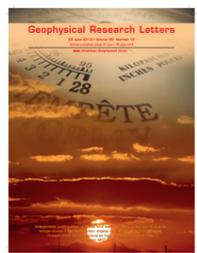
Striolo, Oklahoma  
BES



Smit, LBNL  
BES



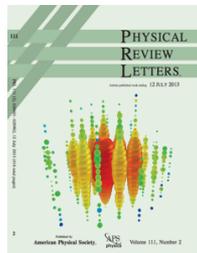
Mei, PNNL  
BES



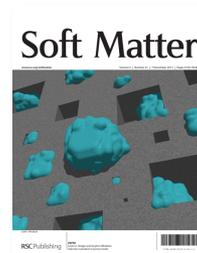
Compo, Colorado  
BER



Persson, LBNL  
BES



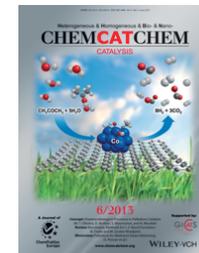
Ha, LBNL  
NP



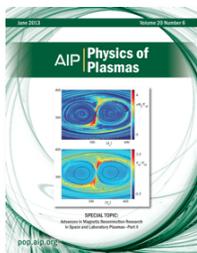
Whitelam, LBNL  
BES



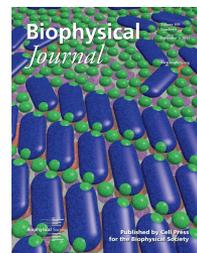
Daggett, Washington  
BER



Mei, PNNL  
BES



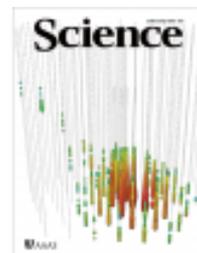
Daughton, LANL  
FES



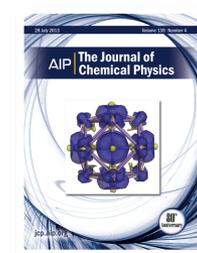
Geissler, UC B  
BES



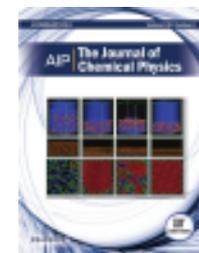
Ghattyvenkatakrishna, FSU  
BER



Ha, LBNL  
NP

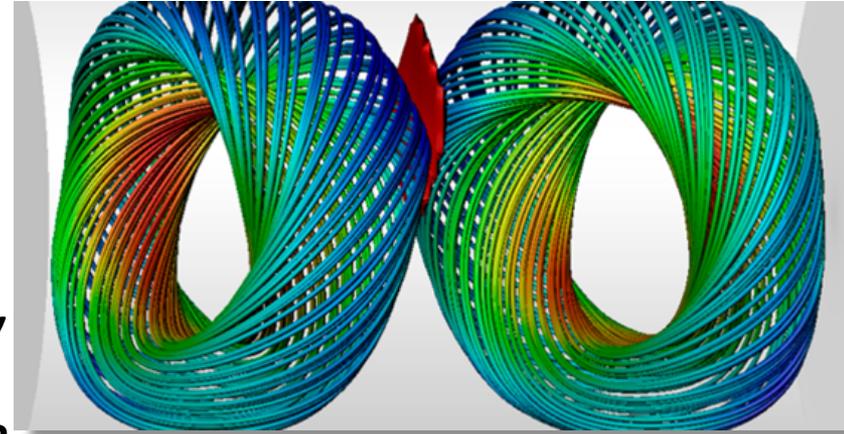


Jena, VCU  
BES



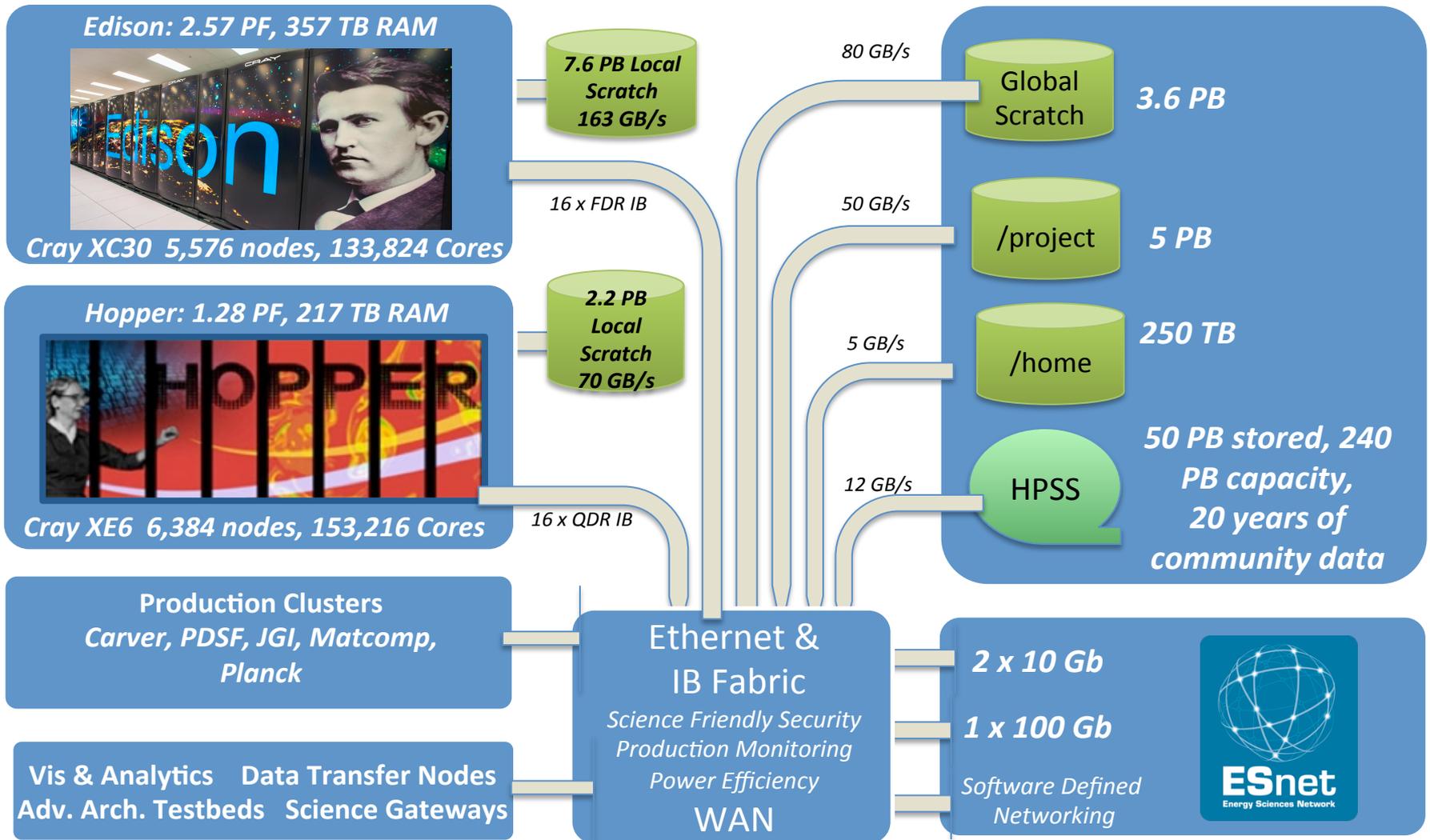
Grest, Sandia  
BES

- 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



**Edison: 2.57 PF, 357 TB RAM**

**Cray XC30 5,576 nodes, 133,824 Cores**

**Hopper: 1.28 PF, 217 TB RAM**

**Cray XE6 6,384 nodes, 153,216 Cores**

**Production Clusters**  
*Carver, PDSF, JGI, Matcomp, Planck*

**Vis & Analytics    Data Transfer Nodes**  
**Adv. Arch. Testbeds    Science Gateways**

**7.6 PB Local Scratch**  
**163 GB/s**

**2.2 PB Local Scratch**  
**70 GB/s**

**Global Scratch**    **3.6 PB**

**/project**    **5 PB**

**/home**    **250 TB**

**HPSS**  
**50 PB stored, 240 PB capacity, 20 years of community data**

**Ethernet & IB Fabric**  
*Science Friendly Security  
Production Monitoring  
Power Efficiency  
WAN*

**2 x 10 Gb**  
**1 x 100 Gb**  
*Software Defined Networking*

# 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**

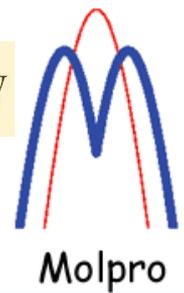
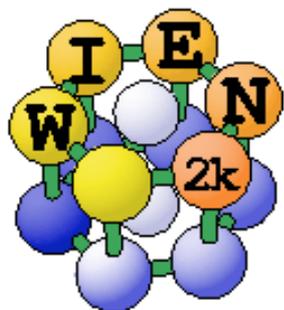
# Simple Rules for Success



- 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.

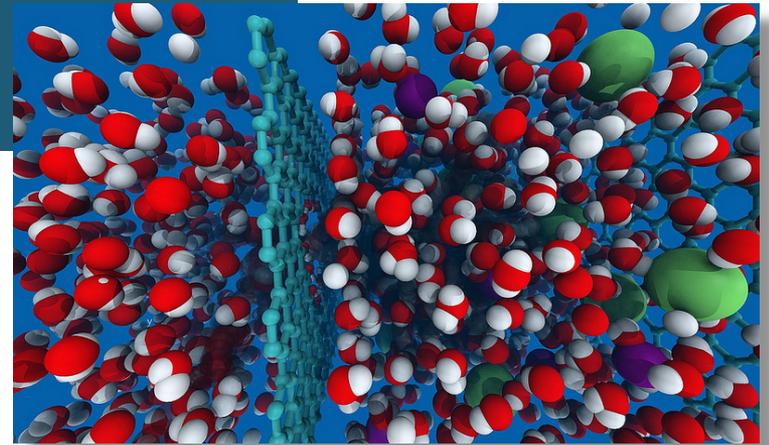


• More than 13.5 million lines of source code Compiled, Optimized, and Tested



- **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.*

**NERSC** **40** YEARS  
at the  
FOREFRONT  
1974-2014



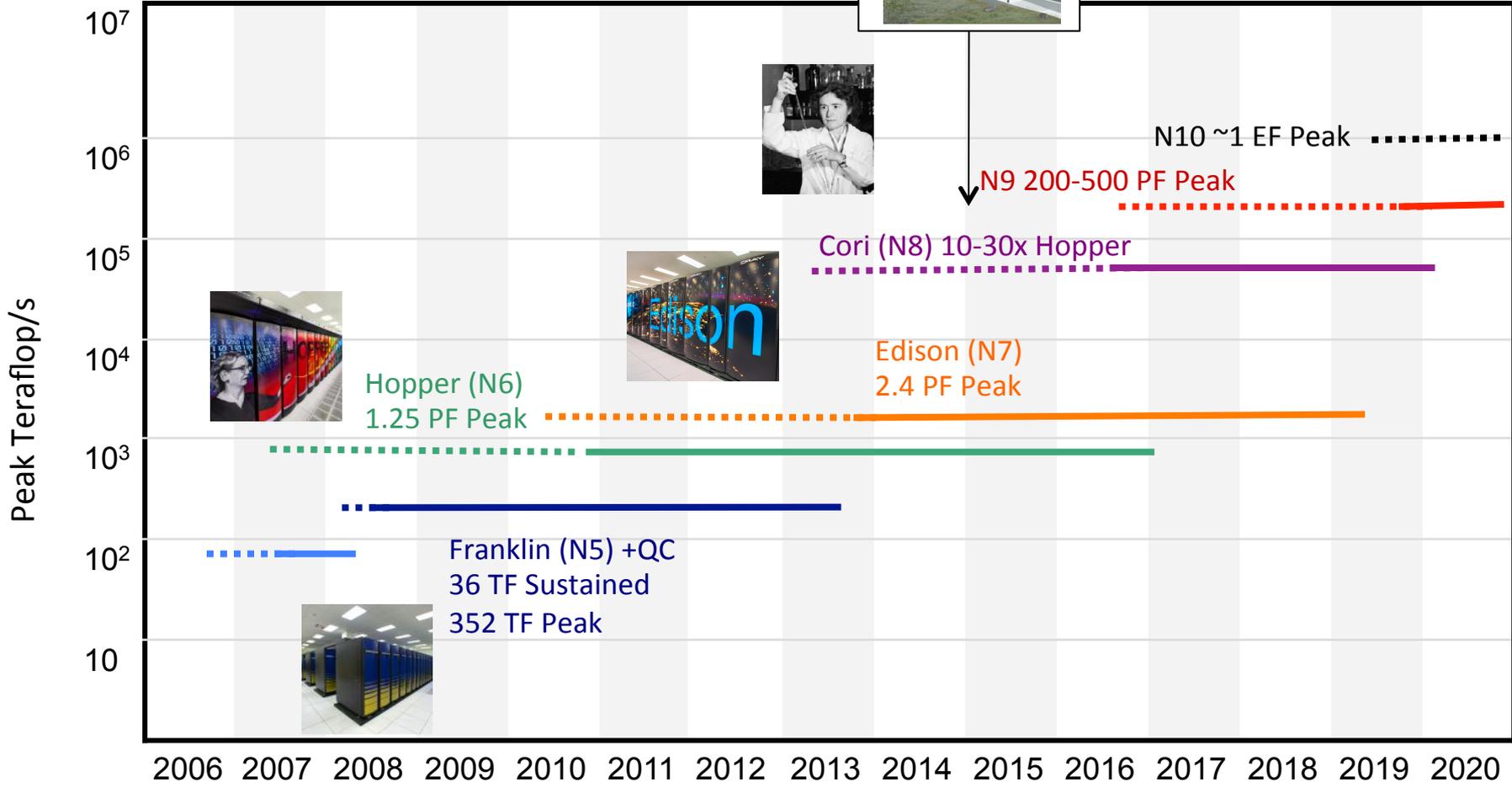
U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# NERSC Roadmap



## CRT Facility



# Change and Consistency



- **NERSC will be physically moving to a new facility in 2015.**
- **Carver will be “retired” August 31, 2015.**
  - Dirac GPU testbed will retire December 12, 2014
- **NERSC-8 will be installed; Disruptive change: codes will likely 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

