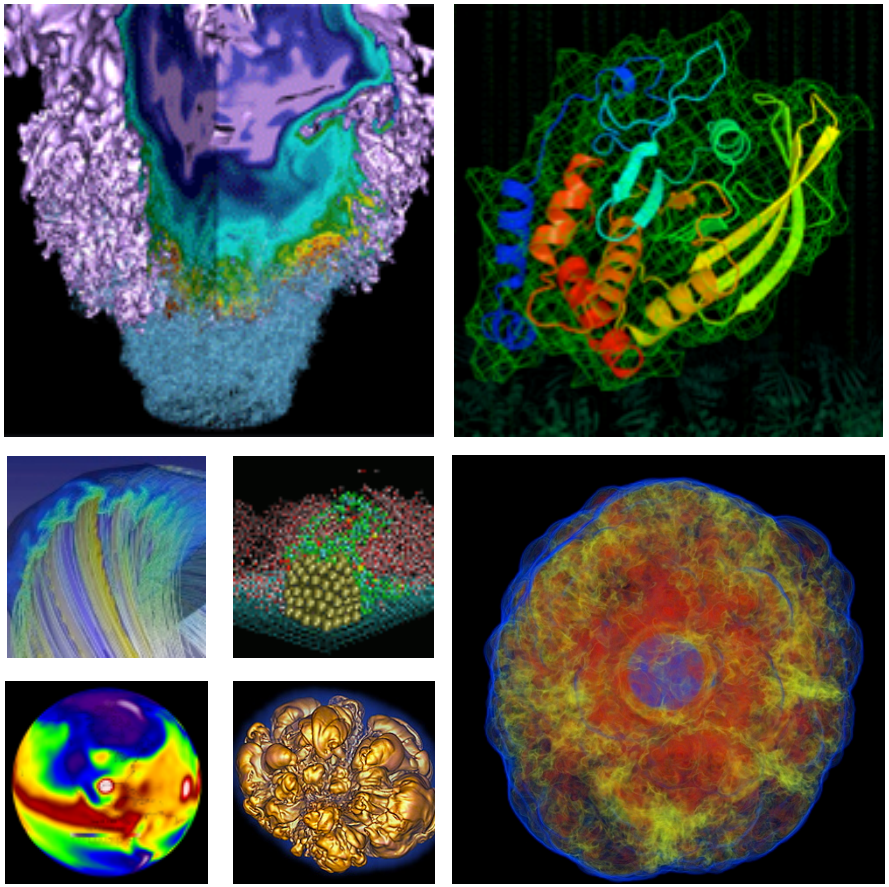
NERSC Overview



NERSC 40 YEARS at the FOREFRONT 1974-2014

Harvey Wasserman
User Services Group

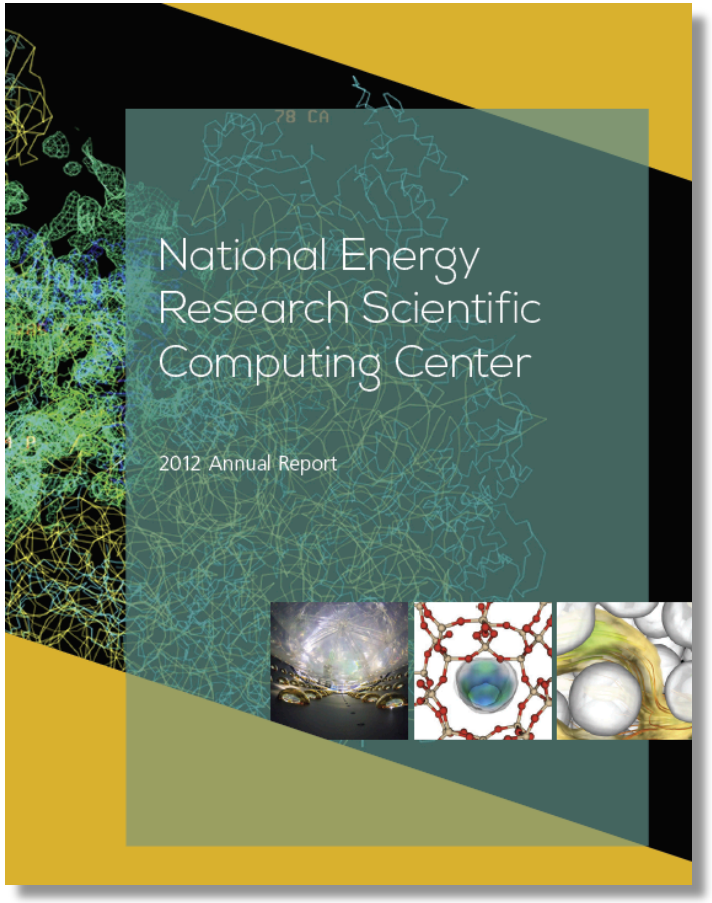
February 3-6, 2014

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB Lawrence Berkeley National Laboratory

NERSC

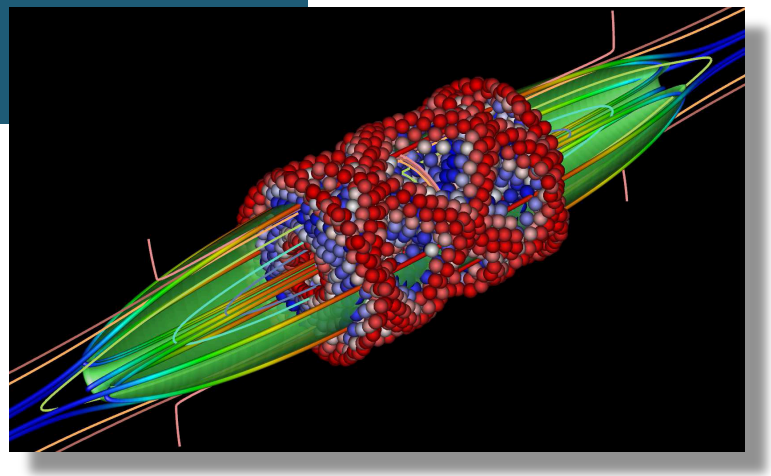
- **National Energy Research Scientific Computing Center**
  - Established 1974, first unclassified supercomputer center
  - Original mission: to enable computational science as a complement to magnetically controlled plasma experiment
- Today's mission: **Accelerate scientific discovery at the DOE Office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



Today's Talk

- **Some simple rules for getting work done at NERSC and a brief introduction to the Center**

Rule # 1: You Are Not Alone



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

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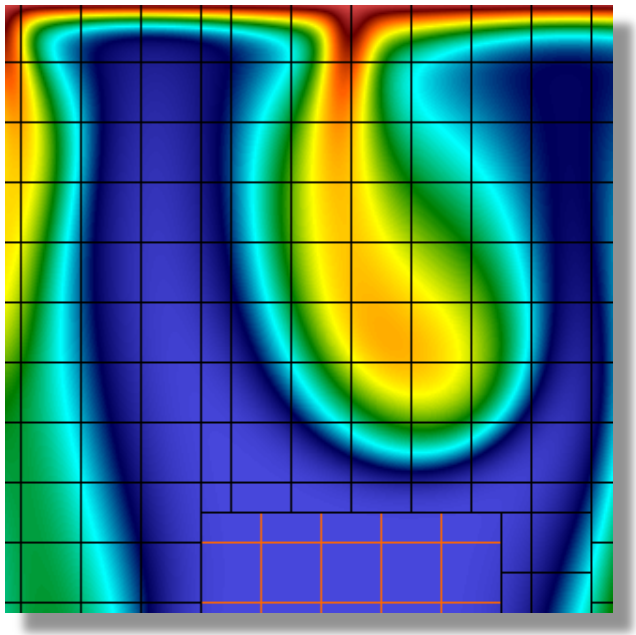
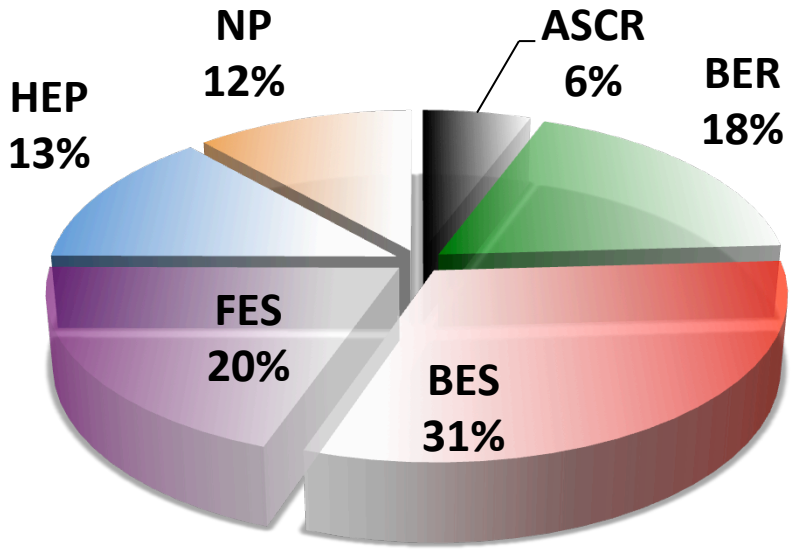
NERSC: Production Computing for the DOE Office of Science

- **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")



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**

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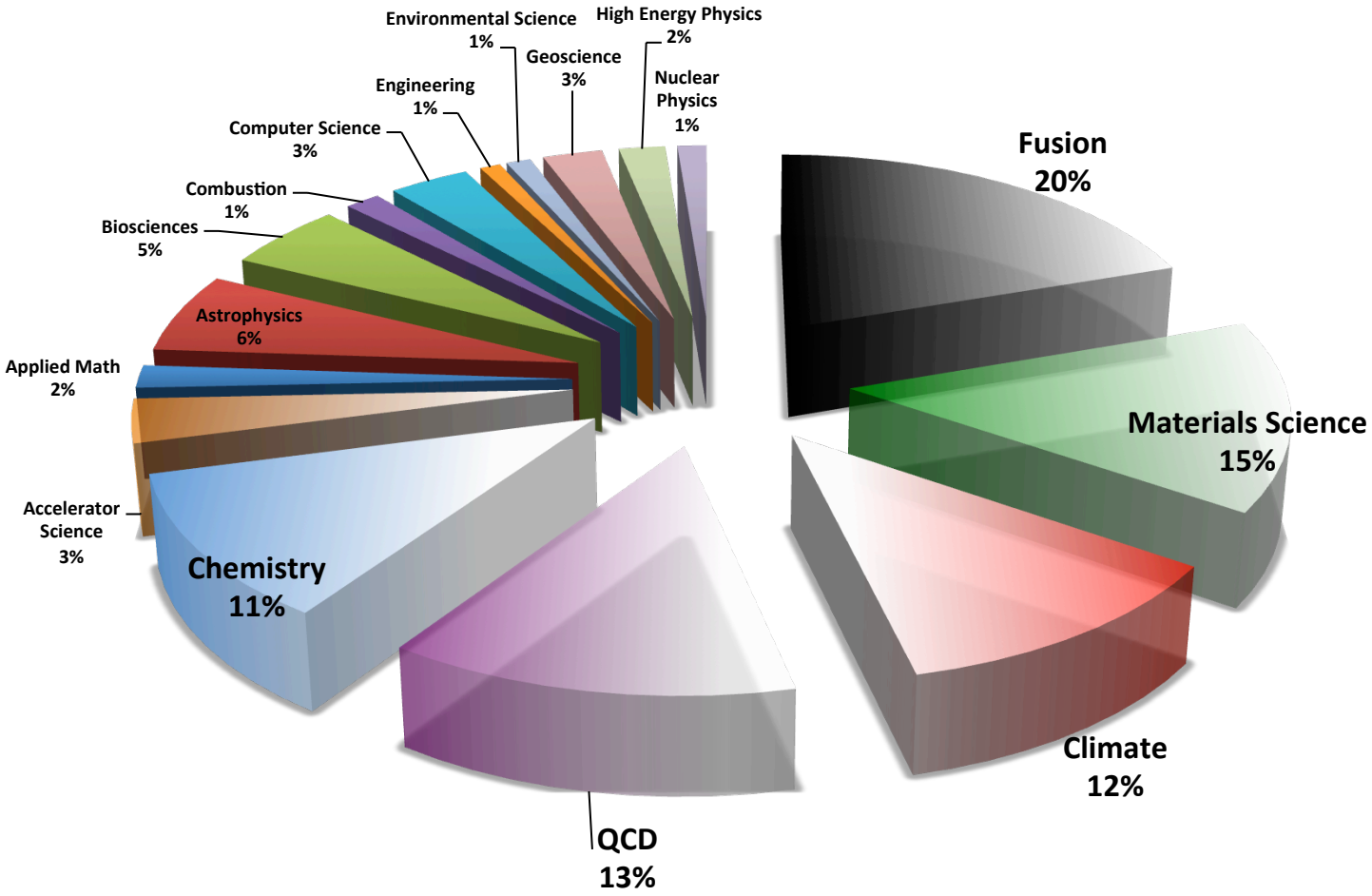
Science View of Workload



NERSC 2013 Allocations By Science Area

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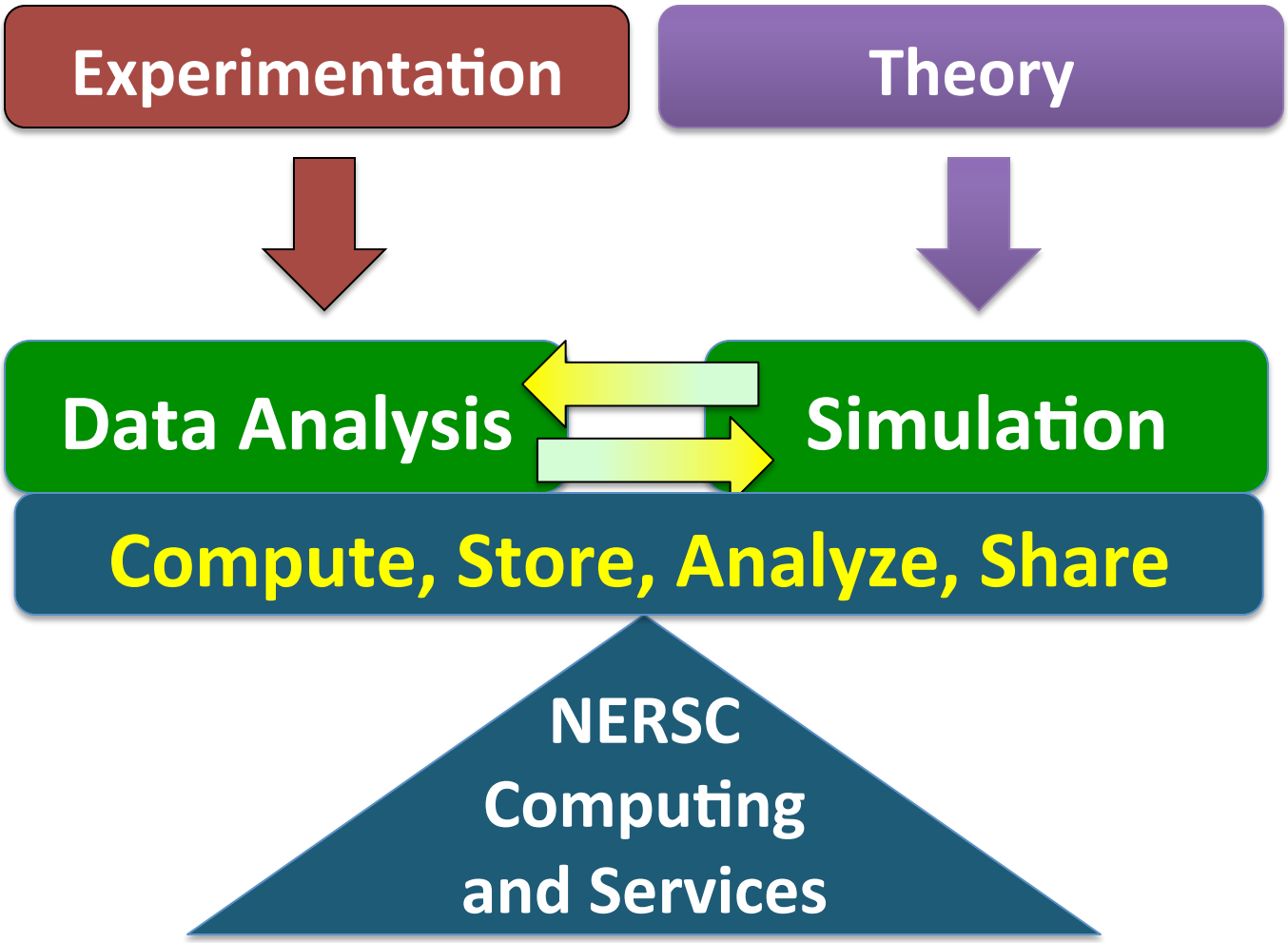
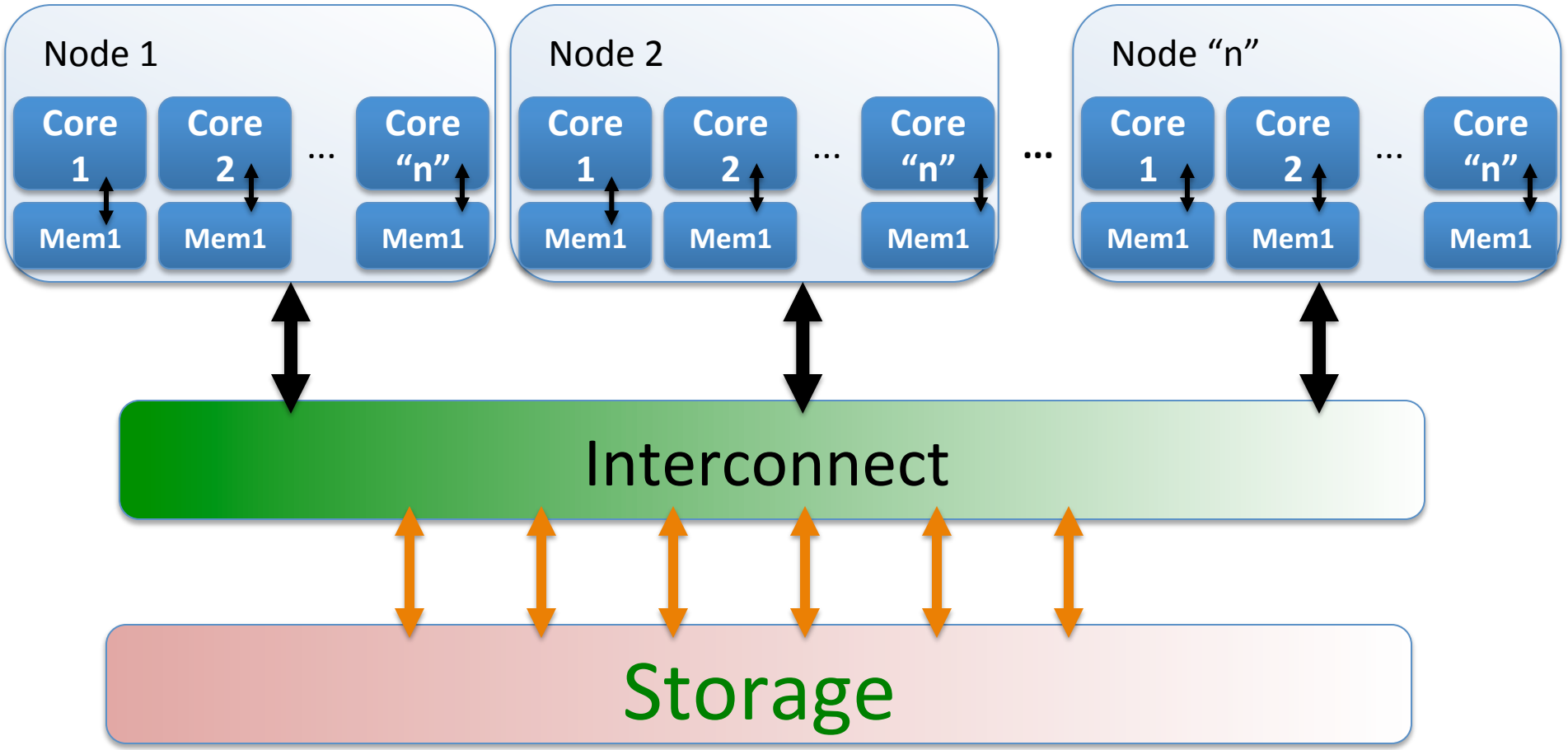
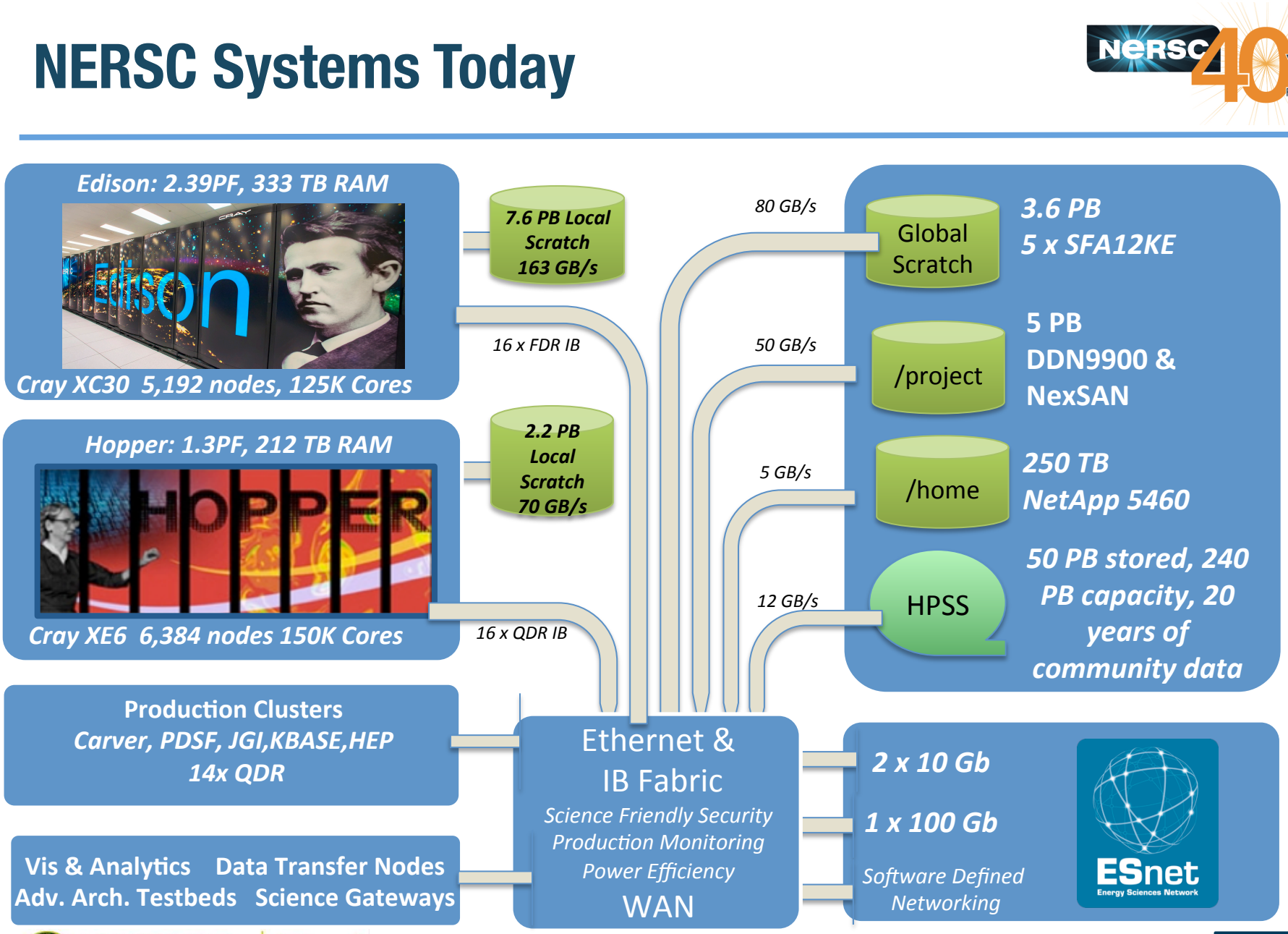
What Role Does NERSC Play?



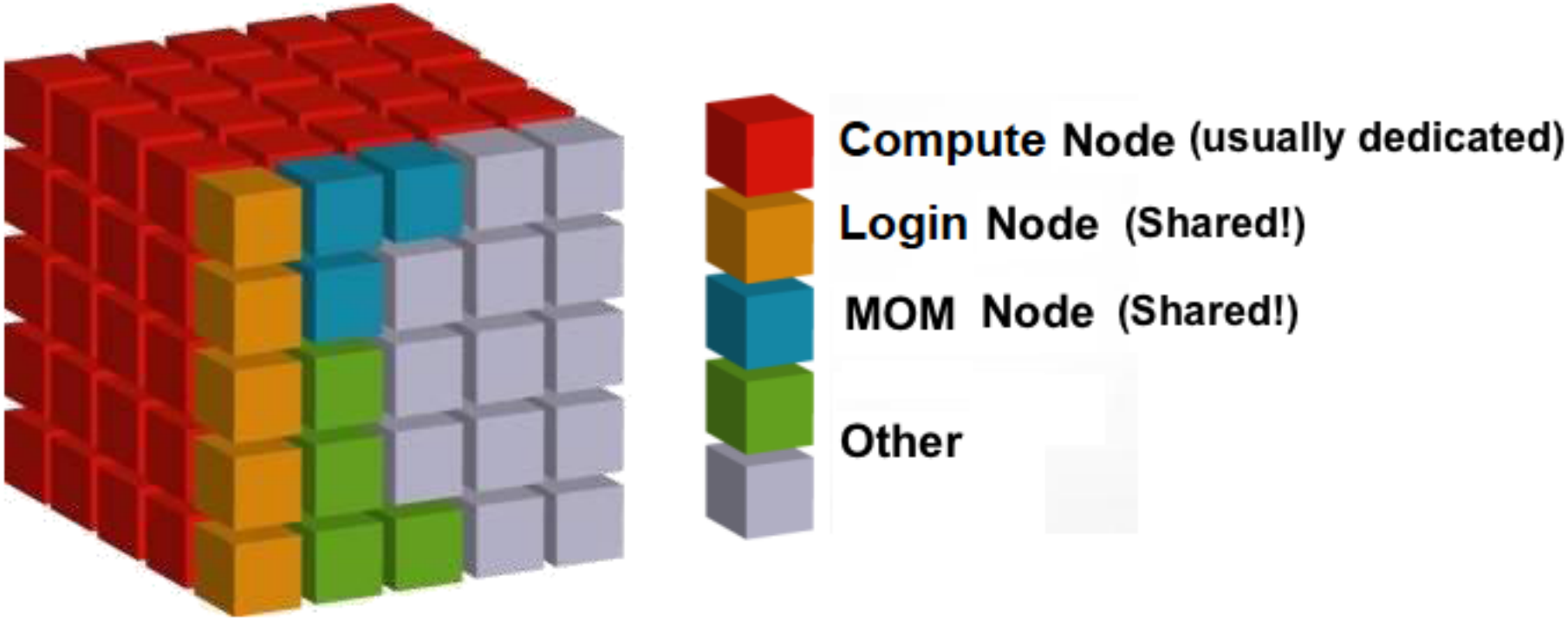
Generic Multiprocessor Architecture



NERSC Systems Today



You Are Not Alone



Usage Model:

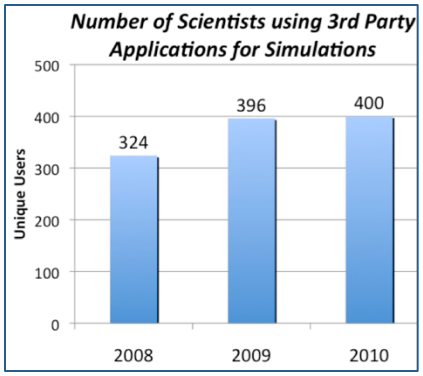
- Connect to Login nodes; edit, transfer, compile, and submit jobs to batch system to access compute nodes
- Compute nodes run applications; do not run codes on login nodes
- Service nodes handle support functions.

Some Sharing Notes

- License limits for some software; make sure to terminate sessions when done
- Use batch system to access compute nodes.
- Run compute-intensive codes on compute nodes
- Limit data transfer or do it on “data transfer” nodes via batch.

Chemistry & Materials Applications

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



A linear-scaling density functional method

Qbox

LAMMPS

NAMD
Scalable Molecular Dynamics

GAMESS

siesta

b-initio

VASP
ackage
ienna
imulation

Q-CHEM

GAUSSIAN

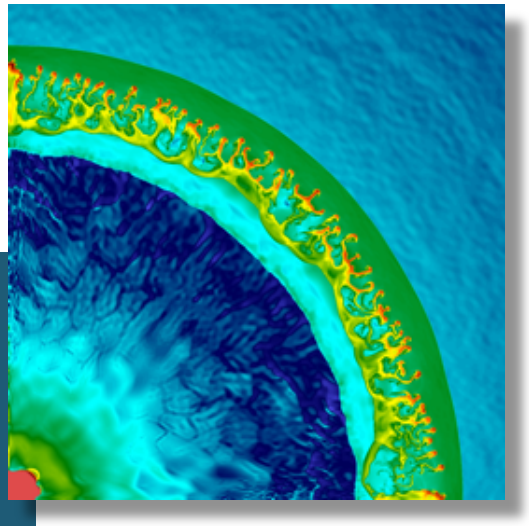
BerkeleyGW

NWCHEM

CPMD

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

Rule # 2: 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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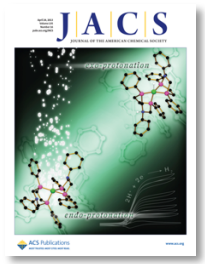
Journal Cover Stories from NERSC-Enabled Research 2013

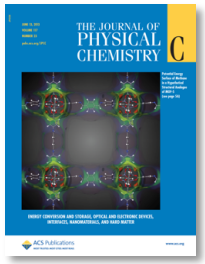
Leung, Sandia
BES

Wu, ColoMines
BES

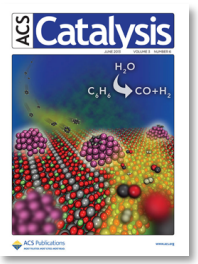


Raugei, PNNL
BES

Striolo, Oklahoma
BES



Smit, LBNL
BES



Mei, PNNL
BES

Compo, Colorado
BER

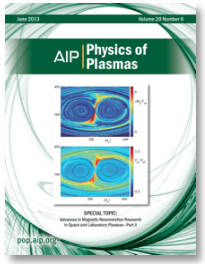
Persson, LBNL
BES

Ha, LBNL
NP

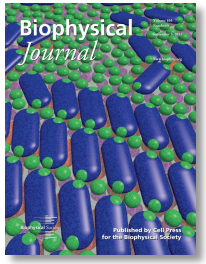
Whitelam, LBNL
BES

Daggett, Washington
BER

Mei, PNNL
BES



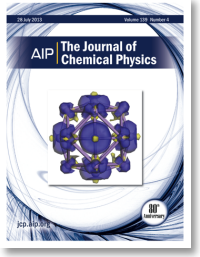
Daughton, LANL
FES



Geissler, UC B
BES

Ghattyvenkatakrishna, FSU
BER

Ha, LBNL
NP



Jena, VCU
BES

Grest, Sandia
BES

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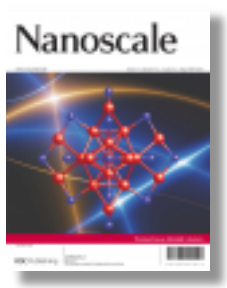
Journal Cover Stories from NERSC-Enabled Research 2012

Devanathan, PNNL: BES



Jiang, ORNL: BES

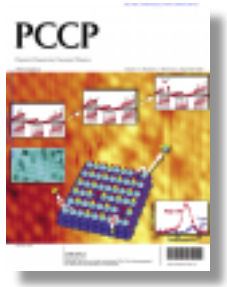
Daggett, U. Washington: BER

Jiang, ORNL: BES

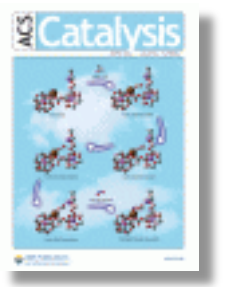
Liang, U. Maryland: BER

Ching, U. M-KC: BES

Dupuis, PNNL: BES

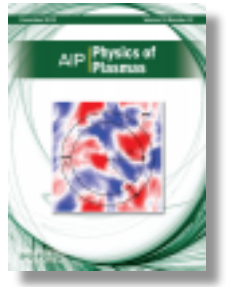


Petrik, PNNL: BES



Snurr, Northwestern: BES

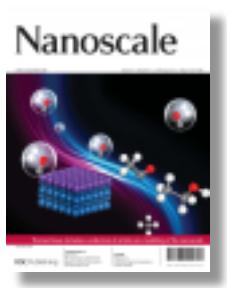
Izzo, GA: FES



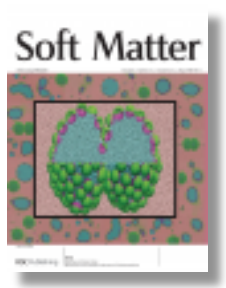
Dorland, U. Maryland: FES

Das, LANL: BES

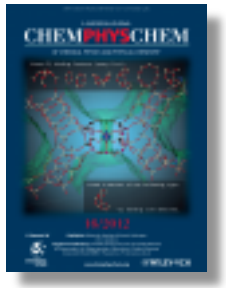
Sugiyama, MIT: FES



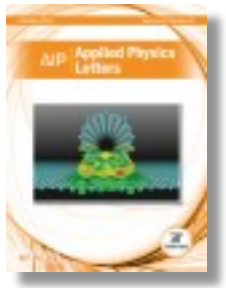
Jiang, ORNL: BES



Striolo, U. Oklahoma: BES



Smit, UCB: BES



Varga, Vanderbilt: BES

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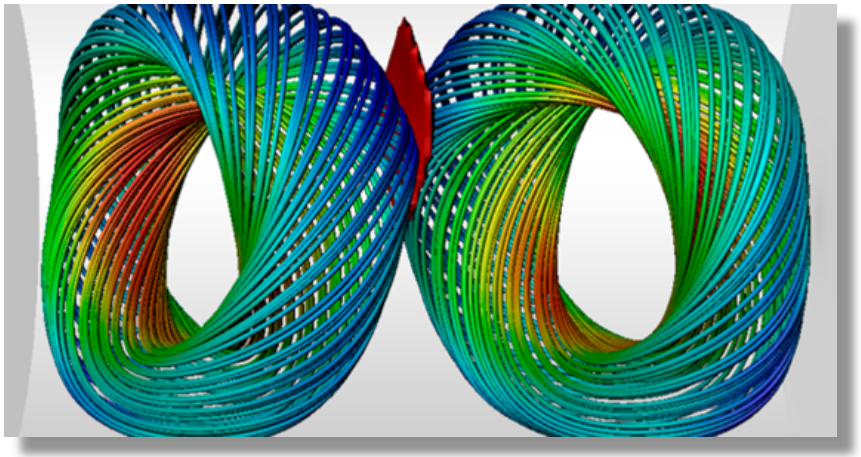
NERSC Users Report ~1,500 Publications / Year

- **Make sure you acknowledge NERSC in publications; please use "official" acknowledgement**

- **Science highlights sent to DOE each quarter.**
  - Send us links to your publications.
  - See http://www.nersc.gov/news-publications/news/
  - See http://www.nersc.gov/news-publications/publications-reports/science-highlights-presentations/
  - See http://www.nersc.gov/news-publications/journal-cover-stories/



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

Simple Rules for Success

- Use our web site
- 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

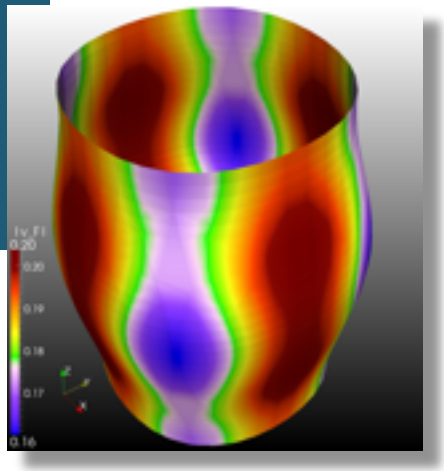
System Choices

- **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**

Rule # 3: (Not Always)



Color map of calculated Fermi Surfaces showing anisotropy of the Fermi velocities ranging from low (blue) to high (red). Image courtesy of Tanmoy Das, Los Alamos National Laboratory. Repo m1245

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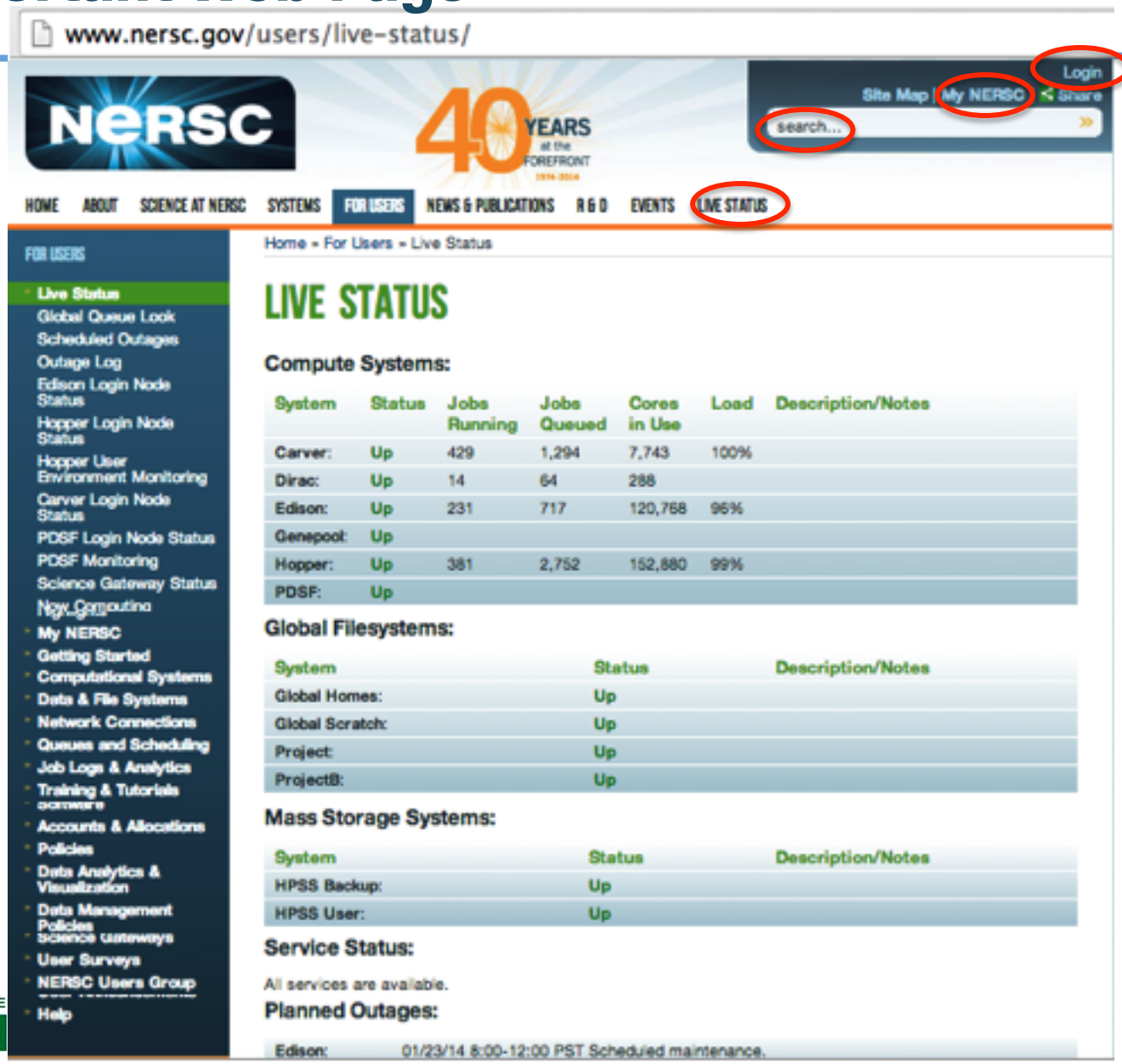
Getting Help

- **Web pages: www.nersc.gov**
  http://www.nersc.gov/users/computational-systems/
- **Submit a ticket: http://help.nersc.gov/**
- **Send e-mail:**
  - HPC Consulting: consult@nersc.gov
  - Account Management: accounts@nersc.gov
- **Call us:**
  - 800-66-NERSC (800-666-3772) or 1-510-486-8600
  - **HPC Consulting = menu option 3**
  - **Account Management = menu option 2**
  - **8-5, M-F Pacific Time**

Getting Help

- **Tips for working with the HPC consultants:**
  - State which machine your question is about.
  - Provide error message(s) if applicable.
  - Provide batch job ID if job crashed
  - Provide filesystem, paths to files
  - Provide your NERSC user ID
  - New issue? New trouble ticket.

Important Web Page



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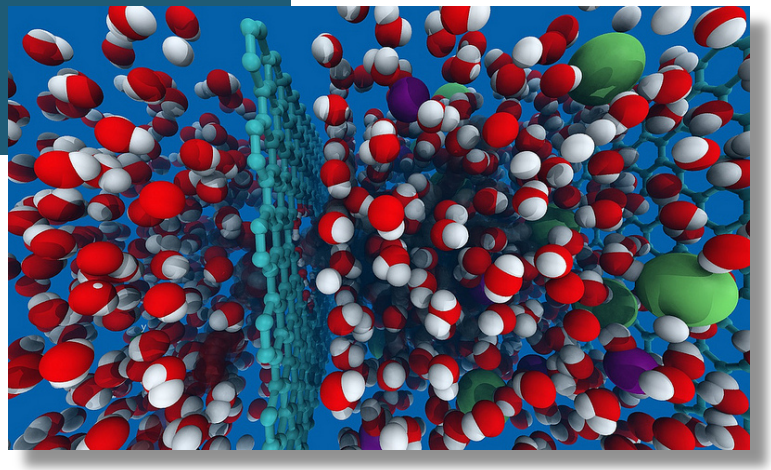
NERSC User's Group

- **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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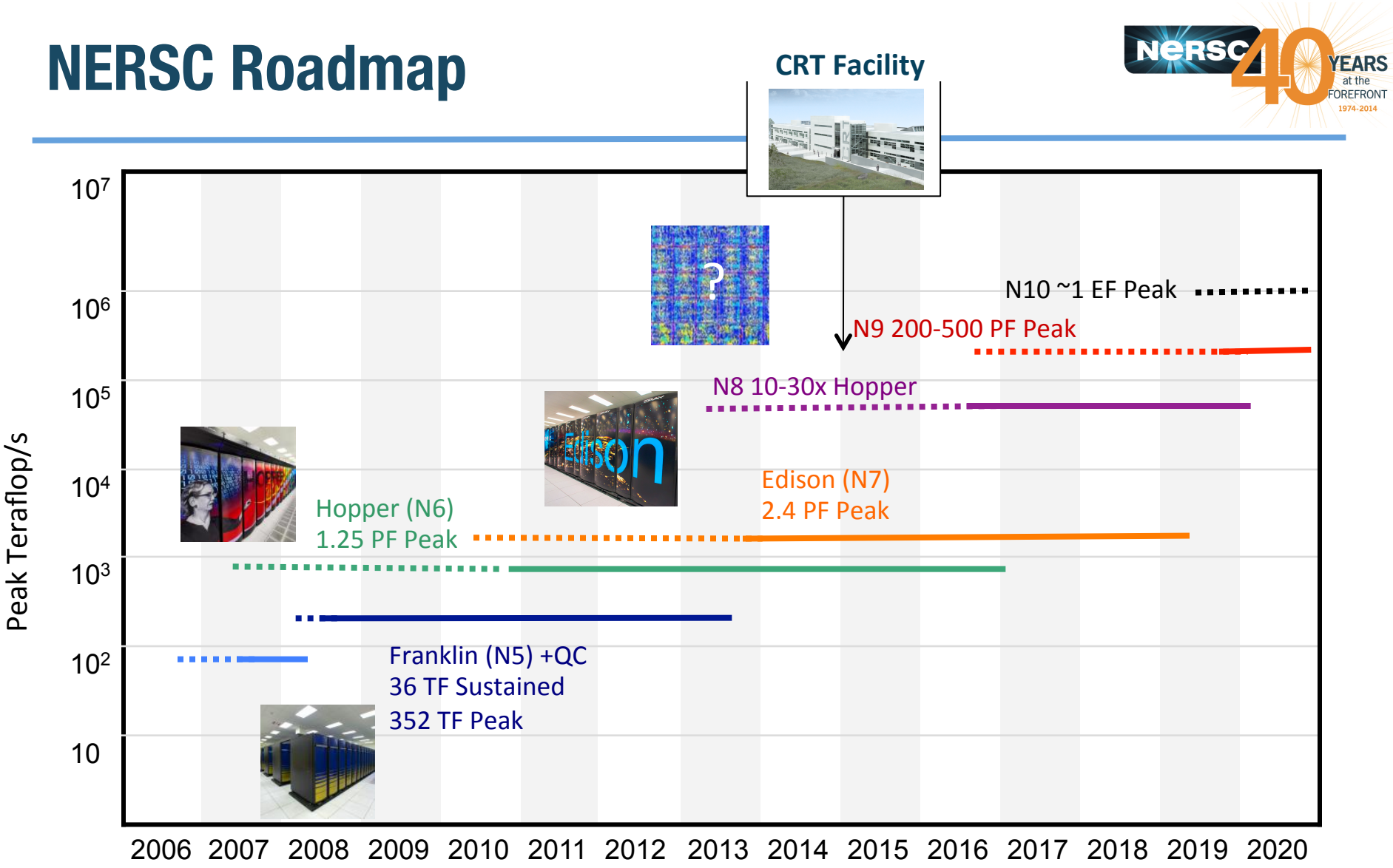
NERSC Roadmap



Change and Consistency

- Future computing systems will likely consist of more energy efficient, highly parallel architectures
- More cores per node; more threads per core; less memory per core; deeper memory hierarchy; more emphasis on loop-level parallelism
- Disruptive change: codes likely need to be modified

- NERSC will help users make this transition

Thank you and welcome to NERSC!