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

*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*
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

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
NERSC 2013 Allocations
By DOE Office

<table>
<thead>
<tr>
<th>DOE Office</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>ASCR</td>
<td>6%</td>
</tr>
<tr>
<td>BER</td>
<td>18%</td>
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<tr>
<td>BES</td>
<td>31%</td>
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<tr>
<td>FES</td>
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<tr>
<td>HEP</td>
<td>13%</td>
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<tr>
<td>NP</td>
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<tr>
<td>ASCR</td>
<td>Advanced Scientific Computing Research</td>
</tr>
<tr>
<td>BER</td>
<td>Biological &amp; Environmental Research</td>
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<td>Basic Energy Sciences</td>
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Science View of Workload

NERSC 2013 Allocations
By Science Area
NERSC Systems Today

**Edison:** 2.57 PF, 357 TB RAM
- Cray XC30
- 5,576 nodes, 133,824 Cores
- Local Scratch 163 GB/s
- 16 x FDR IB
- 7.6 PB Local Scratch
- 80 GB/s

**Hopper:** 1.28 PF, 217 TB RAM
- Cray XE6
- 6,384 nodes, 153,216 Cores
- Local Scratch 70 GB/s
- 16 x QDR IB
- 2.2 PB Local Scratch
- 12 GB/s

**Global Scratch**
- 3.6 PB
- /project
- 50 GB/s
- 5 PB
- /home
- 250 TB
- HPSS
- 50 PB stored, 240 PB capacity, 20 years of community data

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

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

**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**: fast processors; fastest interconnect; best for scaling to large core counts; higher NERSC machine charging factor

- **Hopper**: previous generation processors; excellent scalability; lower charge factor

- **Cori**: newest system, Phase I
Babbage

- Babbage: a NERSC testbed containing the current generation Intel Knight's Corner (KNC) coprocessor
- One login node and 45 compute nodes with two MIC cards
- Each MIC card contains 60 cores, with 4 hardware threads per core and 8 GB of memory per card
- Each core has a 512 KB L2 cache locally with high speed access to all other L2 caches (fully cache coherent).
Logging on to NERSC

```
ssh -X -l train22 edison.nersc.gov
```

(try not to mess up typing your password)

You can go into nim.nersc.gov to change your password, but for now please just use the one you have.

Hopefully with the -X flag you will be have access to x windows applications like emacs for easy editing (depends on your laptop)
Using Edison

- Edison has 12 login nodes. You will be randomly connected to one of those 12 when you ssh to edison.nersc.gov. In all cases it will appear to you as if you are on "edison.nersc.gov."

- The login nodes are where you compile codes, submit jobs, and view data. The login nodes on Edison are "external," meaning they are not directly connected to Edison's internal high-speed "Aries" network. Because the login nodes are external you can log in and work with data and files when the main system is undergoing maintenance.

- Please do not execute long-running applications on the login nodes. Instead, use a batch script and submit it so that the applications run on the Edison compute nodes.
General running: Grabbing an interactive shell

• To run an interactive job on Edison's compute nodes you must request the number of nodes you want and have the system allocate resources from the pool of free nodes. The following command requests 2 nodes using the debug queue.
  ```
edison% qsub -l -q debug -l mppwidth=48
```
• The `-l` flag specifies an interactive job. The `-q` flag specifies the name of the queue and `-l mppwidth` determines the number of nodes to allocate for your job, but not as you might expect. The number of nodes given to your job (remember, the system allocates nodes, not cores), is the value of mppwidth divided by the number of cores per node. On Edison, with 24 cores per node, the number of nodes is mppwidth/24 plus one more if there is a remainder. (Other job directives including the account name [-A repo] can be passed as arguments).
• Assuming there are free nodes, the `qsub` command will log you into a MOM node and return your prompt. You will be in your home directory, but can reference the directory from which you submitted the job as `$PBS_O_WORKDIR`. From the shell prompt, you can start your program on the compute nodes using the "aprun" command.
  ```
edison% cd $PBS_O_WORKDIR edison% aprun -n 48 ./a.out
```
During the SC15 tutorial

- Please grab interactively only one or at most two nodes
- Use our special queue
- \#PBS -W x=FLAGS:ADVRES:Edison.SC15.376253