NERSC Users Group 2013

Warren Focke 2013/02/20

What is NERSC?

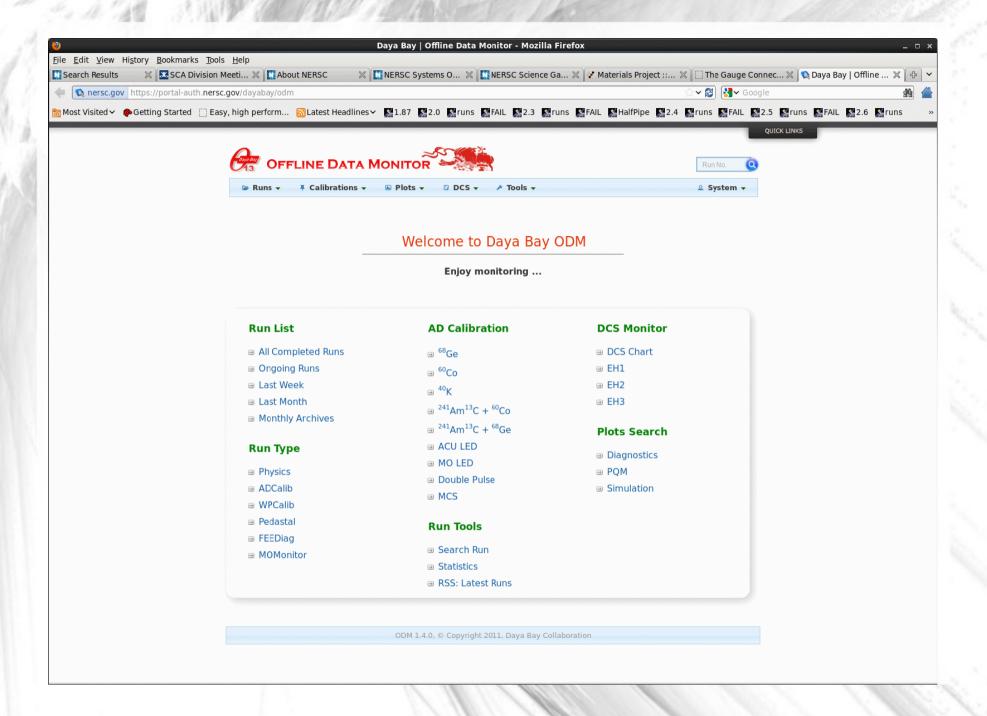
- "The primary scientific computing facility for the Office of Science"
- Main facility is a Cray XE6 with ~150k cores
- Cray XC30 under construction
- IBM dataplex, ~10k cores
 - This is where they've stuck me
 - And I'm fine with that
- Also becoming a data repository

- Supercomputers are very different from batch clusters
 - It's all about the network
 - Scheduling is hard 2-d packing problem
- Focused on MPI
 - Highly parallel
 - They expect you to run on ~1e4 cores
 - For short times ~1hr
- It's common for long jobs to checkpoint & restart

- Do I/O from a single node, distribute via MPI calls
- Monte-Carlo or event reconstruction could run well on this sort of setup
 - It would require some adjustment in thinking
 - And would probably underutilise the network

- They also have some more batch-like systems
 - But you have to pay for those
 - Staff is aware that some classes of users would like to see more of this
- They are will work with customers to customize solutions
- Planck got custom-managed hardware by pledging 2.5 FTEs to use it

- NEWT RESTful API allowing access of NERSC resources through the web
 - Staff has used it to implement a lot of their own management toools
- Users are doing some really cool stuff with it
- Science gateways
 - QCD
 - Astronomy
 - Materials science
 - Climate



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Database Statistics

A Materials Genome Approach

30732 materials

3044 bandstructures

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Latest News

pymatgen v2.5.2

by Shyue Ping Ong - 22 hours ago

Version 2.5.2 of pymatgen has been released! Check out the change log at https://pypi.python.org/pypi/pymatgen for information on the latest changes.

pymatgen v2.5.2

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- LSST DESC was granted 2.5M hours
- Initial use is raytracing the telescope
 - Lots of variation in job runtimes makes it hard to schedule
- Hoping to use NEWT to run pipeline jobs at NERSC, controlled from SLAC
- Will need to set up parallel jobs that act as virtual batch farms
 - e.g. Reserve 32 nodes for 24 hours
 - Use a (somewhat experimental) queueing system taskfarmerMQ