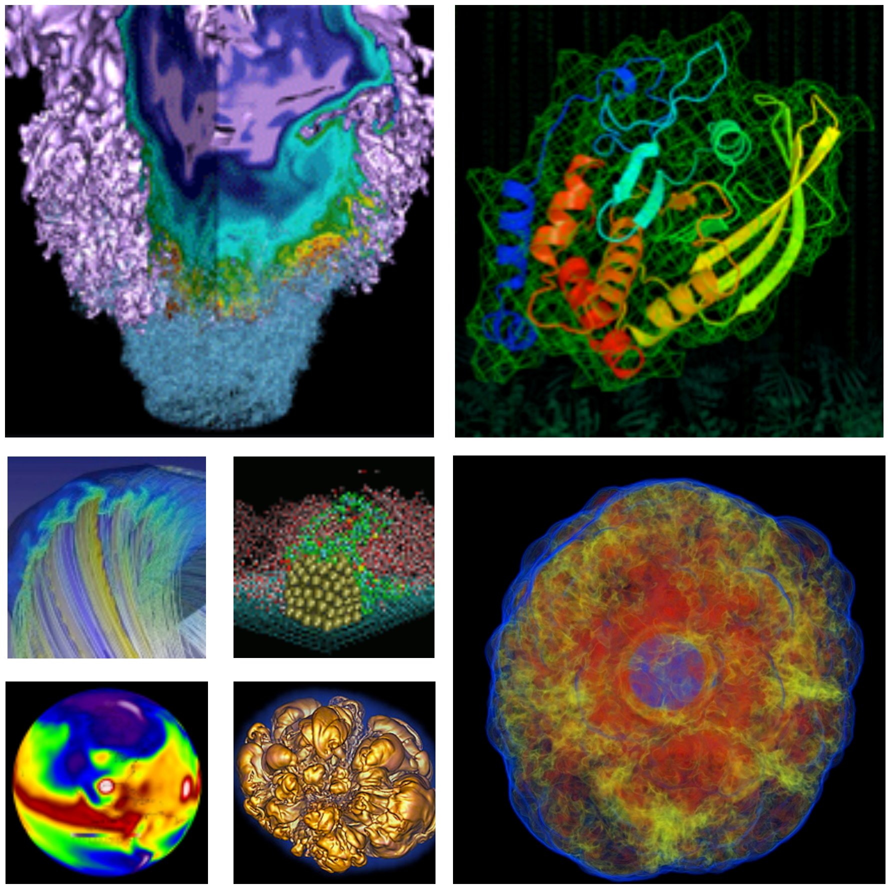
Computing Environment



David Turner

NERSC User Services Group

New User Training
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Node Types

- **Login nodes**
  - Shared
  - Job preparation and submission
- **MOM nodes**
  - Shared
  - Where batch script executes
    - Parallel job launcher
      - Hopper/Edison: aprun
      - Carver: mpirun
- **Compute nodes**
  - Not shared
    - Except serial queue

Login Nodes

- **Edison**
  - Twelve nodes
    - 16 cores, 2.0GHz Intel Sandy Bridge
    - 512GB
- **Hopper**
  - Eight nodes
    - 16 cores, 2.4GHz AMD Opteron
  - Four nodes
    - 32 cores, 2.0GHz AMD Opteron
  - 128GB
- **Carver**
  - Four nodes
    - 8 cores, 2.66GHz Intel Nehalem
    - 48GB

Login Node Access

- Connect (via ssh) to *load balancer*

```
% ssh edison.nersc.gov
% ssh hopper.nersc.gov
% ssh carver.nersc.gov
% ssh genepool.nersc.gov
% ssh pdsf.nersc.gov
```

- **Load balancer selects login node based on:**
  - Number of connections
  - Memory of previous connections from same IP
    - If you login everyday, you'll probably end up on the same login node every time.

Login Node Usage

- **Login nodes are shared by many users, all the time**
- **Edit files, compile programs, submit batch jobs**
- ***Some* post-processing/data analysis**
  - IDL
  - MATLAB
  - NCL
  - python
- ***Some* file transfers**
  - Use data transfer nodes for large/long-running transfers
- **Please use discretion**
  - *All* users get frustrated by sluggish interactive response

Login Node Monitoring

- Determine number of available cores

```
% grep processor /proc/cpuinfo | wc -l
```

- Determine amount of physical memory

```
% grep MemTotal /proc/meminfo
```

- Use “top” command to view process activity

Login Node Guidelines

- Use *no more* than 50% of available cores
- Use *no more* than 25% of available memory
- Limit use of parallel "make"

```
% make -j 4 all
```

- NERSC will kill user processes if response becomes unacceptable
- Terminate idle sessions of licensed software
  - IDL
  - MATLAB
  - Mathematica

Shell Initialization Files

- **Standard dot files**
  - .bashrc, .profile, .cshrc, .login, etc.
  - Symbolic links to read-only files
    - Allows NERSC to provide common environment
- **Personal dot files**
  - Aliases, environment variables, modules, etc.
  - Use .ext suffix (".ext files")
  - .bashrc.ext, .profile.ext, .cshrc.ext, .login.ext, etc.
- **Use "fixdots" to start over**
  - Creates $HOME/KeepDots.<timestamp>
  - Restores all dot files to current default state
  - If PATH corrupted: /usr/common/usg/bin/fixdots
- **Use NIM to change default login shell**

NERSC Supported Software

- **NERSC provides a wide range of software**
  - Scientific Applications
    - VASP, Amber, NAMD, ABySS, ...
  - Compilers
    - PGI, Intel, GCC, Cray
  - Scripting Languages
    - perl, python, R
      - and packages for each!
  - Software Libraries
    - blas/lapack (MKL), boost, hdf5, netcdf, …
  - Utilities
    - gnuplot, git, mercurial, cmake, …
  - Debuggers and Profilers
    - CrayPat, DDT, TotalView, gdb, MAP, darshan
  - Visualization
    - Visit, ParaView, VMD, ...
- **See complete list**

  http://www.nersc.gov/users/software/

Software is Managed by Modules

- **NERSC provides many versions of many software packages**
  - To support diverse workload on systems
- **Maintaining all these separate software installations on heterogeneous systems is a major challenge!**
  - Software can't just be installed in the base operating system
    - How many copies of /usr/bin/vasp could be supported?
  - Each software package installed in its own directory

    /usr/common/usg/blast+/2.2.26

Modules is the user interface to software at NERSC

How to Access NERSC Software

- **Identify the software you need**
  - Use the NERSC website
    http://www.nersc.gov/users/software/
  - Use "module avail"
    - *Lots* of output
    - Each system has different modules!
- **Load the module**

```
% idl
idl: Command not found.
% module load idl
% which idl
/usr/common/usg/idl/idl82/bin/idl
```

Loading Modules

- **Separate modules exist for each version of software**
  - Syntax: <name>/<version>
  - Default provided if no <version> supplied

```
% module avail idl
idl/7.1   idl/8.0   idl/8.2(default)
% module load idl/7.1
```

- **Load modules in every batch script**
  - Ensure correct run-time environment
  - Self-documenting for troubleshooting and reproducibility

Other Useful Module Commands

`module unload <modulename>`

– Remove the module from your environment

`module swap <module1> <module2>`

– Unload one module and replace it with another

```
module swap pgi gcc
```

`module list`

– See what modules you have loaded right now

`module show <modulename>`

– See what the module actually does

`module help <modulename>`

– Get more information about the software

Default Modules

- **When you login, many *default* modules are loaded automatically**
  - Usually foundational modules which are required to get proper function from the system
    - Build environment, required libraries and applications, batch environment
  - Use caution in unloading these
- **Swapping to functionally equivalent module may be OK**

```
carver% module swap pgi gcc
hopper% module swap PrgEnv-pgi PrgEnv-gnu
```

- **Each NERSC system has different default modules**

Types of Modules

- **Applications**
  - VASP, amber, blast, …
  - Usually only set PATH, LD_LIBRARY_PATH
- **Libraries**
  - Set LD_LIBRARY_PATH
    - but probably not on Crays
  - Set “helper” environment variable for building software
    - Header/include file search paths
    - Library search paths
    - Library names

```
% module load hdf5
% mpicc mycode.f $HDF5
```

Cray Programming Environment

- **Compiler specific**

  PrgEnv-pgi, PrgEnv-intel, PrgEnv-cray, PrgEnv-gnu

  – Intel is default on Edison, PGI is default on Hopper

- ***Meta-modules***

  – Organize a set of modules

    - Compiler (intel, pgi, cray, gnu)
    - Libraries (including MPI) tuned for compiler

- **Swapping Programming Environments**

  ```
  module swap PrgEnv-pgi PrgEnv-intel
  ```

  – **swaps compiler**

  – ***no need to swap libraries!***

Carver “Programming Environment”

- **Not as sophisticated as Cray PrgEnv**
- **Separate compiler and OpenMPI modules**

Compiler module	OpenMPI module
pgi	openmpi
intel	openmpi-intel
gcc	openmpi-gcc

- ***Must keep libraries consistent with compiler!***

Compiler Wrappers

- **Edison/Hopper**
  - Defined by PrgEnv modules
  - `ftn`, `cc`, `CC`
  - Provides include and library search paths for MPI and some common math libraries (e.g., Cray's libsci)
  - Provides consistent level of optimization across compilers
- **Carver**
  - Defined by openmpi modules
  - `mpif90`, `mpicc`, `mpiCC`
  - Provides include and library search paths for OpenMPI
- **Seldom need native compilers!**

Resources

http://www.nersc.gov/users/software/nersc-user-environment/

http://www.nersc.gov/users/software/nersc-user-environment/modules/

http://www.nersc.gov/users/computational-systems/edison/programming

/http://www.nersc.gov/users/computational-systems/hopper/programming/

http://www.nersc.gov/users/computational-systems/carver/programming/

NERSC 40 YEARS at the FOREFRONT

Thank you.