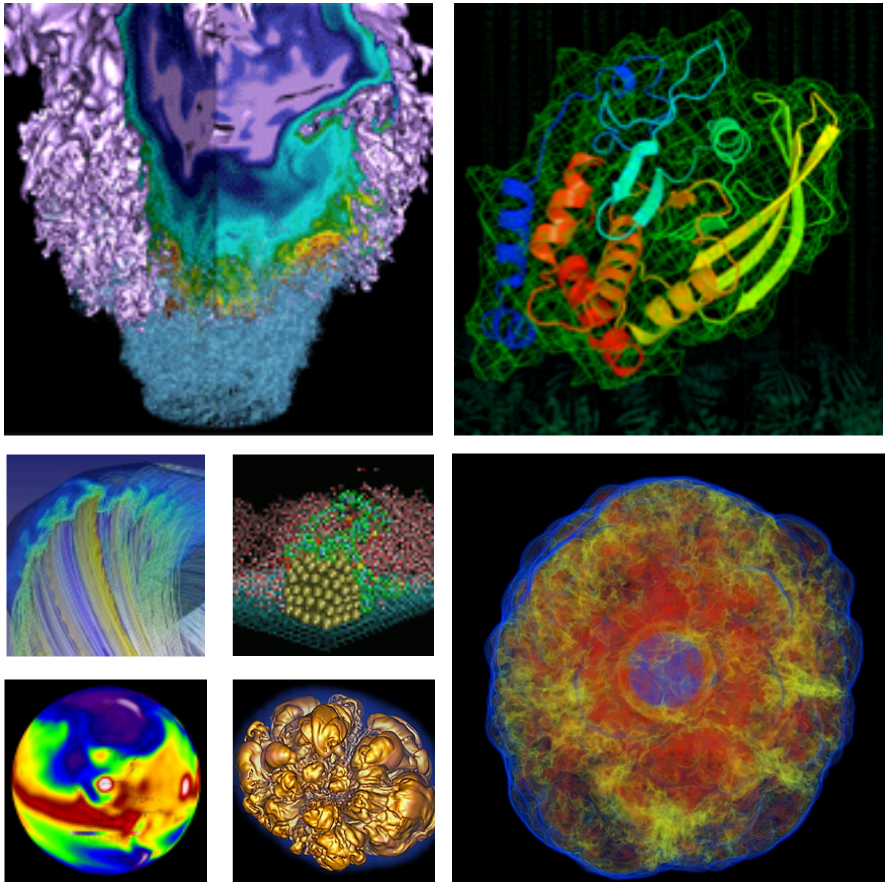
Computing Environment



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New User Training
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NERSC 40 YEARS at the FOREFRONT 1974-2014
U.S. DEPARTMENT OF ENERGY | Office of Science
BERKELEY LAB Lawrence Berkeley National Laboratory

Node Types

- **Login nodes**
  - Shared with other users
  - Code compilation, job preparation and submission
- **Compute nodes**
  - Not shared (except shared queue on Cori)
- **Service nodes**
  - File system access (lustre), data movement (HPSS), network connections to outside world, etc.
  - Not accessed directly

Login Node Configuration

- **Edison**
  - **Twelve** nodes
    - 16 cores, 2.0 GHz Intel Sandy Bridge, **512 GB**
- **Cori**
  - **Twelve** nodes
    - 16 cores, 2.0 GHz Intel Sandy Bridge, **512GB**
- **Genepool**
  - Four nodes
    - 8 cores, 2.3 GHz Intel Sandy Bridge, 32 GB
- **PDSF**
  - Three nodes
    - 16 cores, 2.6 GHz Intel Sandy Bridge, 125 GB

Login Node Access

- Connect (via ssh) to *load balancer*

```
% ssh edison.nersc.gov
% ssh cori.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

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, etc.
- ***Some* file transfers**
  - Use data transfer nodes for large/long-running transfers (dtn[01-04].nersc.gov)
- **Please use discretion**
  - *All* users get frustrated by sluggish interactive response
  - If unsure, please write to *consult@nersc.gov*

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 32 all
```

- **NERSC will kill user processes if login nodes become unacceptably slow or unresponsive**
- **Terminate idle sessions of licensed software**
  - IDL
  - MATLAB
  - Mathematica

Shell Initialization Files

- **Standard dot files are maintained by NERSC**
  - `.bashrc`, `.profile`, `.cshrc`, `.login`, etc.
  - Symbolic links to read-only files
- **Personal dot files**
  - Aliases, environment variables, modules, etc.
  - Use .ext suffix (".ext files") `.bashrc.ext`, etc.
- **Broken? Use "`fixdots`" to start over**
  - Creates `$HOME/KeepDots.<timestamp>`
  - Restores all dot files to 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
    - Intel, GCC, PGI, Cray
  - Scripting Languages
    - perl, python, R - including common packages for each
  - Software Libraries (some maintained by Cray)
    - blas/lapack (MKL), boost, hdf5, netcdf, …
  - Development utilities
    - git, mercurial, cmake, …
  - Debuggers and Profilers
    - CrayPat, DDT, TotalView, gdb, MAP, darshan, IPM, VTune
  - Visualization
    - Visit, ParaView, VMD, ...
- **See complete list**
  - `$ module avail`
  - http://www.nersc.gov/users/software/

Software is Managed by Modules

- **Identify the software you need**
  - Use the NERSC website

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

- **Load the module**

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

Loading Modules

- **Different module 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

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 PrgEnv-intel PrgEnv-gnu
```

`module list` **-- Very useful!**

- See what modules you have loaded right now

`module show <modulename>` **-- Very useful!**

- 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**

```
edison% module swap PrgEnv-intel PrgEnv-gnu
```

Types of Modules

- **Applications**
  - VASP, amber, blast, …
  - Usually only set `PATH`, `LD_LIBRARY_PATH`
- **Libraries**
  - Set `LD_LIBRARY_PATH`
  - Set "helper" environment variable for building software
    - Header/include file search paths (e.g. `C_INCLUDE_DIR`)
    - Library search paths (e.g. `PETSC_DIR, HDF5, PYTHONPATH`)
    - `module show` command useful here

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

Module pitfalls

- Output from `module <command>` is piped to STDERR, and **not** STDOUT
- Need to re-direct output if you need to pipe to another command
  - `module list 2>&1 | grep dmapp`
- Need to be re-loaded for each newly spawned shell (unless specified in setup scripts)
- No inverse mapping from library name to module
- Most popular packages are pre-packaged by Cray and have "cray-" prepended to their names
  - `cray-petsc` instead of `petsc`
  - `cray-netcdf` instead of `netcdf`
  - `cray-hdf5-parallel` instead of `hdf5-parallel`

Cray Programming Environment

- **Compiler specific**

  PrgEnv-intel, PrgEnv-cray, PrgEnv-gnu (modules)

  – Intel is default on Edison and Cori

- **Swapping Programming Environments**

  ```
  module swap PrgEnv-gnu PrgEnv-intel
  ```

  – **swaps compiler**

  – ***no need to swap libraries!***

Compiler Wrappers

- **On Cori / Edison:**
  - Defined by `PrgEnv-*` modules
  - `ftn` (Fortran), `cc` (C), `CC` (C++)
  - Provides include header and library search paths for MPI, common math libraries (e.g., `cray-libsci`), Cray system software
  - Provides consistent level of optimization across compilers
- **Seldom need native compilers!**

(`ifort, icc, gcc, g++` etc)

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/cori/programming/

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Thank you.

CHOS Environment

- **Provides different OS environments**
  - – Often different third-party software
    - Some software packages have specific OS requirements
      - – Possibly due to validation requirements
- **Used on Genepool and PDSF**
- **Transparent**
  - – Default configuration for most users
  - – Alternate configurations for some users
- **Details on website**

http://www.nersc.gov/users/computational-systems/pdsf/software-and-tools/chos/

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

Software is Managed by Modules

- **NERSC provides many versions of many software packages**
- **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/vasp/5.3.5

Modules is the user interface to software at NERSC

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!***