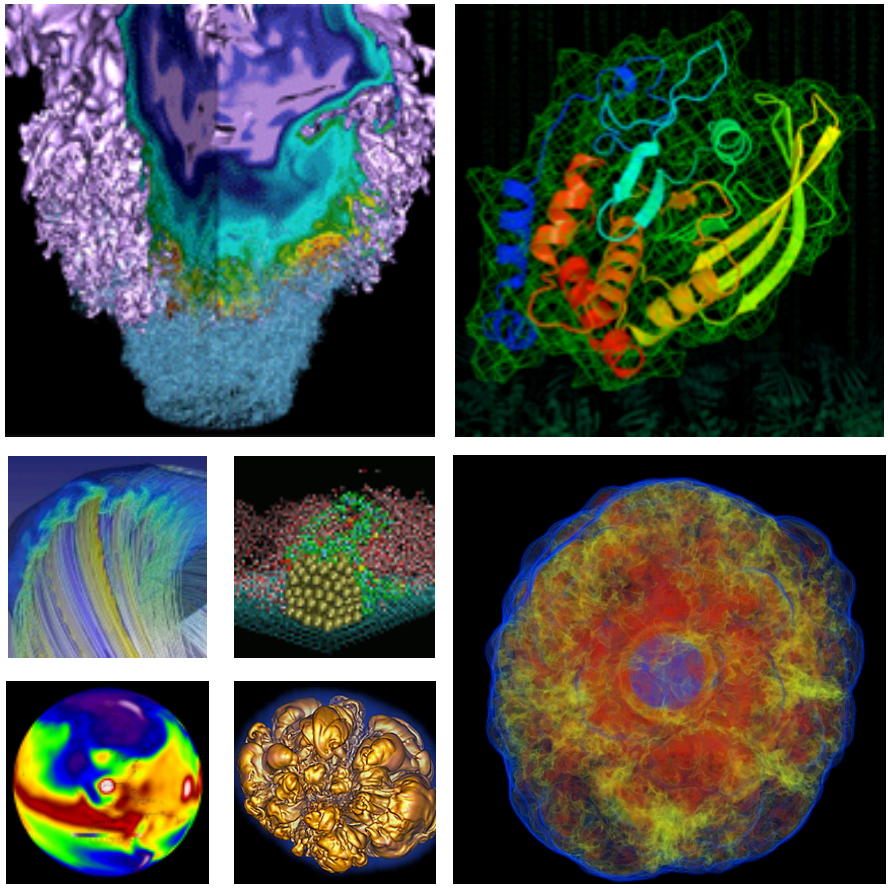
Using Modules at NERSC



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NERSC Supported Software

- **NERSC provides a wide range of scientific and computer programming software to users**
  - 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, 7zip, cmake, ...
  - Debuggers & 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
    - E.g., /usr/common/usg/blast+/2.2.26

Modules is the user interface to the software at NERSC

How to access NERSC Software

1. Identify the software you need

- Use the NERSC website: http://www.nersc.gov/users/software/
- Use "module avail"

```
[dmj@cvrsvc03 ~]$ module avail

------------------------------------------------ /usr/share/Modules/modulefiles ------------------------------------------------
dot         module-cvs  module-git  module-info modules     null        use.own

--------------------------------------------- /usr/common/usg/Modules/modulefiles ---------------------------------------------
OFEDgcc4.7.0/2.0-2.0.5-Mellanox(default) hdf5-parallel/1.8.3-intel                openmpi-gnu/1.6
R/2.10.1                                 hdf5-parallel/1.8.9-gnu                  openmpi-gnu/1.6.3
R/2.12.0                                 hdf5-parallel/1.8.9-intel                openmpi-gnu/1.6.5
R/2.12.1(default)                        hdfview/2.6.1(default)                   openmpi-intel/1.4.2
R/2.13.1                                 hmpp/2.4                                 openmpi-intel/1.4.3
R/2.14.1                                 hmpp/2.5.1(default)                      openmpi-intel/1.4.5(default)
R/2.15.2                                 htop/1.0.2(default)                      openmpi-intel/1.6
R/3.0.1                                  hwloc/1.6(default)                       openmpi-intel/1.6.3
abinit/6.0.3                             hwloc/1.6.2                              openmpi-intel/1.6.5
abinit/6.10.3                            hwloc-gcc/1.6(default)                   openmpi_ofed2/1.6.5(default)
abinit/6.10.3-gpu                        hwloc-gcc/1.6.2                          openmpi_ofed2-gcc/1.6.5(default)
abinit/6.12.1                            hwloc-intel/1.6(default)                 openmpi_ofed2-intel/1.6.5(default)
abinit/6.12.1-gpu                        hwloc-intel/1.6.2                        openmpi_tcp_only/1.6.5(default)
abinit/6.12.1-magma                      idl/7.1                                  openmpi_tcp_only-gcc/1.6.5(default)
abinit/6.2.2                             idl/8.0                                  openmpi_tcp_only-intel/1.6.5(default)
abinit/6.4.1(default)                    idl/8.2(default)                         oracle-jdk/1.6.0_39_32bit
adios/1.4.0(default)                     idl/bout                                 oracle-jdk/1.6.0_39_64bit
allineatools/4.0-31457                   intel/11.1                               oracle-jdk/1.6.0_41_32bit
allineatools/4.1-32296(default)          intel/12.1.3                             oracle-jdk/1.6.0_41_64bit
allineatools/4.1-32834                   intel/13.0.1(default)                    oracle-jdk/1.6_32bit
. . .
```

Each NERSC system has different Modules!

How to access NERSC Software

2. Load the module

```
[dmj@cvrsvc03 ~]$ which sander
sander: Command not found.
[dmj@cvrsvc03 ~]$ module load amber
[dmj@cvrsvc03 ~]$ which sander
/usr/common/usg/amber/11/bin/sander
[dmj@cvrsvc03 ~]$
```

3. Load the module in your batch script

edison/hopper

```
#!/bin/tcsh -l
#PBS -l walltime=1:00:00
#PBS -l mppwidth=48

module load amber
cd $PBS_O_WORKDIR
aprun -n 48 pmemd ...
```

carver

```
#!/bin/tcsh -l
#PBS -l walltime=1:00:00
#PBS -l nodes=7:ppn=8

module load amber
module load openmpi
cd $PBS_O_WORKDIR
mpirun pmemd ...
```

Load a specific version

- Separate modules exist for each version of the software
- Syntax: <name>/<version>
- Each module has a “default” version if you only request the <name>

Default

module load R

Specific

module load R/3.0.1

```
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R/2.13.1                                 hmpp/2.4                                 openmpi-intel/1.4.3
R/2.14.1                                 hmpp/2.5.1(default)                      openmpi-intel/1.4.5(default)
R/2.15.2                                 htop/1.0.2(default)                      openmpi-intel/1.6
R/3.0.1                                  hwloc/1.6(default)                       openmpi-intel/1.6.3
abinit/6.0.3                             hwloc/1.6.2                              openmpi-intel/1.6.5
abinit/6.10.3                            hwloc-gcc/1.6(default)                   openmpi_ofed2/1.6.5(default)
abinit/6.10.3-gpu                        hwloc-gcc/1.6.2                          openmpi_ofed2-gcc/1.6.5(default)
abinit/6.12.1                            hwloc-intel/1.6(default)                 openmpi_ofed2-intel/1.6.5(default)
abinit/6.12.1-gpu                        hwloc-intel/1.6.2                        openmpi_tcp_only/1.6.5(default)
abinit/6.12.1-magma                      idl/7.1                                  openmpi_tcp_only-gcc/1.6.5(default)
abinit/6.12.2                            idl/8.0                                  openmpi_tcp_only-intel/1.6.5(default)
abinit/6.4.1(default)                    idl/8.2(default)                         oracle-jdk/1.6.0_39_32bit
adios/1.4.0(default)                     idl/bout                                 oracle-jdk/1.6.0_39_64bit
allineatools/4.0-31457                   intel/11.1                               oracle-jdk/1.6.0_41_32bit
```

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

e.g., module swap pgi gcc # on carver

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 ssh to a NERSC system many modules are already loaded for you.**
- **These are usually foundational modules which are required to get proper function from the system.**
  - Use caution in unloading these
  - Swapping to equivalent functionality module may be OK.
    - e.g., module swap pgi gcc # carver
    - e.g., module swap PrgEnv-pgi PrgEnv-gnu #hopper
- **Default modules include build environment, required libraries and applications, scheduler modules**

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

Types of Modules at NERSC

- **Basic software Modules (Applications)**
  - VASP, amber, blast, …
  - Usually only set PATH, LD_LIBRARY_PATH
  - Just for running software
- **Software Library Modules**
  - Set LD_LIBRARY_PATH (mostly on carver/pdsf/genepool)
  - Set a helper environment variable for building software
  - e.g., the 'fftw' module set $FFTW to enable include and linking paths; cc myprog.c $FFTW
- **Programming Environment Modules**

Programming Environment Modules

- **PrgEnv modules are really *meta-modules* which organize a community of modules**
- **These are prevalent on the Cray systems, used to manage the compiler (wrapper) and libraries**
  - Mike will cover this in a minute
- **Loading the PrgEnv-<compiler> module, also loads:**
  - A compiler module (gcc, pgi, intel)
  - Many software library modules with paths tuned for that compiler
- **Swapping a PrgEnv module will attempt to keep the environment consistent (will reload all the library modules)**
  - e.g., module swap PrgEnv-pgi PrgEnv-gnu

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