

Introduction to Modules at CHPC

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Overview of Talk

- Why Modules
- Where to find information
- How to setup to use modules
- Module basics
- Advanced Modules
- Demonstration



What modules do

 Modules are a way of managing the user environment in an interactive session or a batch job



Why Modules

- Modules lets users dynamically change the environment – including easily adding and removing directories needed for a given task from \$PATH etc – without needing to log out and back in
- Easy to switch between version of a package or application – again without having to start a new session
- Useful when packages have conflicts in their environment settings



Module Documentation at CHPC

- https://www.chpc.utah.edu/documentation/software/modules.p hp
- https://www.chpc.utah.edu/documentation/software/modulesadvanced.php
- Video -- https://www.youtube.com/watch?v=Cu6C5INLDAY

We make use of TACC's LMOD

- https://www.tacc.utexas.edu/research-development/taccprojects/lmod
- LUA based



All accounts automatically use modules -

- This is done via the login scripts CHPC provides all accounts, even if you have older dot files
- CHPC uses modules to set up environments upon login: chpc/1.0



Recommendations & Helpful Hints

- Keep both the cshell and bash versions of provided login scripts in your home directory
- DO NOT make changes in the .tcshrc and .bashrc
- Use the .custom.csh/.custom.sh to load modules for programs regularly used in ssh sessions
- Use .aliases file to create aliases but do not set other environment variables in this file; if this file exists it will be sourced during login
- The software database mentions which installations have modules – if there is one you would like us to create, let us know!

Basic Module commands

- module shows the list of module commands
- module load <name> loads module name (shortcut: ml <name>)
- module unload <name> unloads module name (ml -<name>)
- module avail shows a list of "available" modules (ml av)
- module list shows a list of loaded modules (ml)
- module help prints help for the module command
- module help <name> prints help for module
- module show <name> prints the module file
- module purge unload all modules
- module reset system resets to system default (only chpc module loaded)
- module swap <name1> <name2> swaps between two modules



CHPC Module Organization

Core

 Contains modules for applications independent of both the compiler and MPI implementation

Compiler

 Contains modules for applications dependent on a compiler (& version) but not on a MPI implementation

MPI

 Contains modules for applications dependent on both a compiler and a MPI implementation

Modules themselves are named by application name/version



Other Information

- Cannot have multiple compilers loaded
 - If you have intel loaded, and load any gcc it will unload intel
 - As a result we no longer have compiler tag as part of the module name in libraries and applications that are compiler dependent (ex – mpich, openmpi, netcdf, fftw)
- Parallel versions of boost, HDF5 have separate modules
 - hdf5 for module for serial build, phdf5 for module for parallel build
 - boost for serial, phoost for parallel



Default, aliases, and hidden modules

- For some applications have a default module one that is installed if you do not provide a specific version
 - typically the latest version is specified to be the default
- For some modules, especially those with long version names, there is also an alias defined
 - ml intel/17 loads the default 2017 intel
 - ml intel/17.0 loads the 2017.0.098 version
- With move to CentOS7 we have depreciated older installations and their modules so some have been hidden
 - module --show_hidden avail



Module avail command

- module avail shows all modules available based on already loaded module
 - This also marks default (D), already loaded (L), and aliases
- Some modules are dependent on other modules based on organization
 - these modules are not listed unless the modules they depend on are loaded



Module spider command

- module spider shows all modules, including modules that aren't available
- Use module spider <string> to see a subset of modules with string in name, and how to either load the module or how to get more detailed information on how to load



Module show command

- Format module show modulename/version
- Shows you the content of the module file
- This is useful if there is information on running the program included in the module



Advanced Modules

- Users can create "save lists" for commonly needed environments
- Users can write and use their own modules, creating modules for their own installations
- Contact CHPC if you need assistance doing this

Getting Help

- CHPC website
 - www.chpc.utah.edu
 - Getting started guide, cluster usage guides, software manual pages, CHPC policies
- Service-Now issue/incident tracking system
 - Email: <u>helpdesk@chpc.utah.edu</u>
- Help Desk: 405 INSCC, 581-6440 (9-5 M-F)
- We use chpc-hpc-users@lists.utah.edu for sending messages to users