

Introduction to Modules at CHPC

Anita Orendt

Assistant Director

Research Consulting & Faculty Engagement

anita.orendt@utah.edu

14 June 2018

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.php>
- <https://www.chpc.utah.edu/documentation/software/modules-advanced.php>
- Video -- <https://www.youtube.com/watch?v=Cu6C5INLDAY>

We make use of TACC's LMOD

- <https://www.tacc.utexas.edu/research-development/tacc-projects/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 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 avail**)
- **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

Recent Changes

- No longer allowed to 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, pboost 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: helpdesk@chpc.utah.edu
- Help Desk: 405 INSCC, 581-6440 (9-5 M-F)
- We use chpc-hpc-users@lists.utah.edu for sending messages to users; also have Twitter accounts for announcements -- @CHPCOutages & @CHPCUpdates