Introduction to Modules at CHPC

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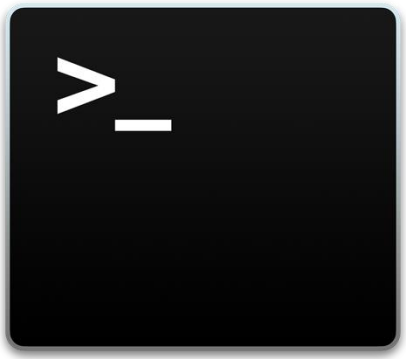
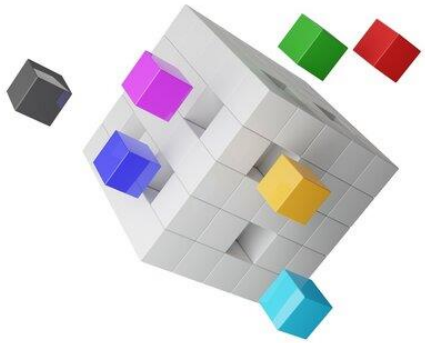
Overview of Talk

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

What modules do

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





Why Modules

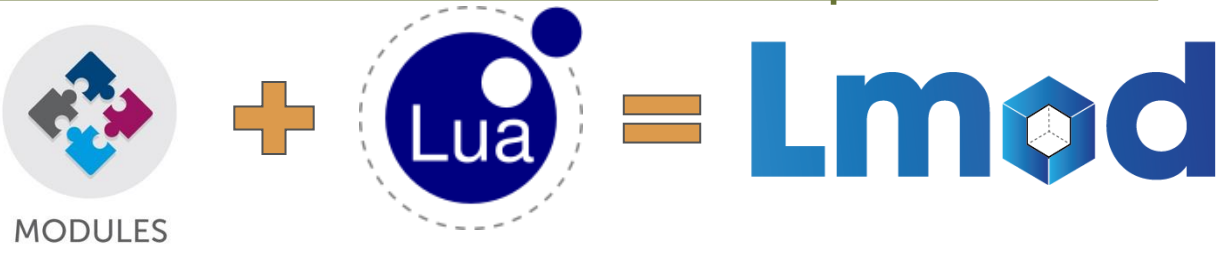
- Modules lets users dynamically change the Shell Environment – including easily adding and removing directories needed for a given task from system **Environment Variables**, eg **$PATH**, without needing to log out and back in
- Easy to switch between version of a package or application – again without 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://youtu.be/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 (dot files) CHPC provides in home directories, even if you have older versions
- **DO NOT** make changes in the **.tcshrc** and **.bashrc**
- Use the **.custom.csh/.custom.sh** to customize environment variables and/or pre-load modules for programs regularly used in ssh sessions
- Use **.aliases** file to create aliases (but not environment variables); if this file exists it will be sourced during login
  - `alias c='clear'`
- You may reset login scripts (dot files) if necessary
  - CHPC official version: /uufs/chpc.utah.edu/sys/modulefiles/templates

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 (lua)
- **module purge** - unload all modules
- **module reset system** – resets to system default
- **module swap <name1> <name2>** - swaps between two modules
- **module spider <string>** - shows all modules that have string in name

Explore CHPC Modules

- **module list (ml)** – see what are currently loaded

```
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)

  Where:
   S:  Module is Sticky, requires --force to unload or purge
```

- **Naming Convention** <ModuleName>/<ModuleVersion>
- **module load <name>/<version>** -- load a module
  - **module load <module1> <module2> …<moduleN>**

```
[class99@linuxclass:~]$ module load matlab/R2022a
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)   2) matlab/R2022a

  Where:
   S:  Module is Sticky, requires --force to unload or purge



[class99@linuxclass:~]$ which matlab
/uufs/chpc.utah.edu/sys/installdir/matlab/R2022a/bin/matlab
```

Explore CHPC Modules (cont.)

- **module purge** – unload all modules

```
[class99@linuxclass:~]$ module purge
```

```
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)
```

```
[class99@linuxclass:~]$ which matlab
/usr/bin/which: no matlab in (/uufs/chpc.utah.edu/sys/bi
al/sbin:/usr/sbin)
```

- **Load a default module** (not specify the version)

```
[class99@linuxclass:~]$ module load matlab
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)   2) matlab/R2023b

  Where:
   S:  Module is Sticky, requires --force to unload or purge



[class99@linuxclass:~]$ which matlab
/uufs/chpc.utah.edu/sys/installdir/matlab/R2023b/bin/matlab
```

Module Avail command

- **module avail (ml av)** – what modules are currently loadable
  - Not an exhaustive list of modules at CHPC
  - Show Loadable modules at the moment
    - Standalone
    - Dependent modules are already loaded in current environment
  - List may change when other modules get loaded or unloaded
  - Marks default (D), already loaded (L), gpu specific (g) and aliases
  - Pagination: module --redirect avail | more
  - Filter: module avail <string>
    - Eg: module avail mat

```
masurca/3.3.1
mathematica/12.3.1
mathematica/13.3.1
mathematica/14.0.0            (D)
matlab/R2021b
matlab/R2022a
matlab/R2022b
matlab/R2023a
matlab/R2023b                 (L,D)
maven/3.3.3
maxquant/1.6.10.43
medaka/1.5.0                  (g)
medaka/1.6.1                  (g)
medaka/1.7.2                  (g,D)
medea/3.7.2
mega2/6.0.0
megadetector/4.1
megalodon/2.3.3
mercurial/3.6
merlin/1.1.2
mesa/r15.14.0
```

CHPC Module Hierarchy

- Core
  - Contains modules for applications independent of both Compiler and MPI modules installed by CHPC (eg self-contained software)
- Compiler
  - Contains modules for applications dependent on a Compiler (& version) module but not on a MPI module
- MPI
  - Contains modules for applications dependent on both a compiler module and a MPI module

Modules themselves are named by application name/version

Module Avail command (cont.)

- module load gcc/8.5.0 → module av

```
---- /uufs/chpc.utah.edu/sys/modulefiles/spack/linux-rocky8-x86_64/Compiler/li
nux-rocky8-nehalem/gcc/8.5.0 ----
   boost/1.77.0                        mpich/4.1.2
   cantera-pokitt/develop              mvapich2/2.3.6          (D)
   cdo/2.0.5                  (D)      mvapich2/2.3.7
   fftw/2.1.5                          netcdf-c/4.8.1
   fftw/3.3.10                (D)      netcdf-cxx/4.2
   gdal/3.3.2                 (D)      netcdf-fortran/4.5.3
   geant4/10.7.3                       openblas/0.3.18
   geant4/11.0.3              (D)      openkim-models/2021-01-28
   gsl/2.7                    (D)      openmpi/4.1.1           (L)
   hdf4/4.2.15                (D)      openmpi/4.1.3-gpu       (g)
   hdf5/1.10.7                         openmpi/4.1.3
   hoomd-blue/2.5.0-gpu-mkl   (g)      openmpi/4.1.4           (D)
   hoomd-blue/2.5.0-gpu-obl   (g,D)    openmpi/4.1.5-gpu       (g)
   hysplit/5.2.3                       openmpi/4.1.5
   intel-mpi/2019.10.317               openmpi/4.1.6-gpu       (g)
   intel-oneapi-mkl/2021.4.0           openmpi/4.1.6
   intel-oneapi-mkl/2022.0.2           py-numpy/1.19.5-mkl
   intel-oneapi-mkl/2022.2.1           py-numpy/1.19.5-obl
   intel-oneapi-mpi/2021.1.1  (D)      py-numpy/1.19.5
   intel-oneapi-mpi/2021.2.0           py-numpy/1.21.3-p38
```

- module load openmpi/4.1.1 → module av

```
---- /uufs/chpc.utah.edu/sys/modulefiles/spack/linux-rocky8-x86_64/MPI/linux-r
ocky8-nehalem/gcc/8.5.0/openmpi/4.1.1 ----
   hdf5/1.8.22      hypre/2.23.0        parallel-netcdf/1.12.2
   hdf5/1.10.7      lammps/20220107     petsc/3.16.4
   hyphy/2.5.41     netcdf-c/4.8.1      wi4mpi/3.5.0
```

Module Avail command (cont.)

- module load hdf5/1.10.7 → which h5diff

```
[class99@linuxclass:~]$ module load hdf5/1.10.7
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)   2) gcc/8.5.0   3) openmpi/4.1.1   4) hdf5/1.10.7

  Where:
   S:  Module is Sticky, requires --force to unload or purge



[class99@linuxclass:~]$ which h5diff
/uufs/chpc.utah.edu/sys/spack/linux-rocky8-nehalem/gcc-8.5.0/hdf5-1.10.7-fcupy
pb7a7hytf7lwlba7sgwx6hkenyv/bin/h5diff
```

- Note: For a specific application (<name>/<version>), there might be multiple module instances, each was installed with different compilers and/or mpi implementations --- For reproducibility, take notes on the **target module** as well as the **dependent modules**.

Module Spider command

- Most of the time, we want to do direct searches
  - Is a module installed on CHPC?
  - What versions do you have?
  - How do I load it? (what dependencies needed?)
- **module spider <string>**

  - show all versions

```
[class99@linuxclass:~]$ module spider hdf5

----------------------------------------
  hdf5:
----------------------------------------
     Versions:
        hdf5/1.8.19
        hdf5/1.8.22
        hdf5/1.10.7
        hdf5/1.12.2
        hdf5/1.14.1-2
     Other possible modules matches:
        phdf5
```

module spider <name>/<version>

- show how to load a specific module

```
[class99@linuxclass:~]$ module spider hdf5/1.10.7

----------------------------------------------------------------------------
  hdf5: hdf5/1.10.7
----------------------------------------------------------------------------

    You will need to load all module(s) on any one of the lines b
he "hdf5/1.10.7" module is available to load.

      gcc/11.2.0  openmpi/4.1.6
      gcc/11.2.0-cpu  openmpi/4.1.6
      gcc/11.2.0-gpu  openmpi/4.1.6
      gcc/8.5.0
      gcc/8.5.0  intel-oneapi-mpi/2021.4.0
      gcc/8.5.0  openmpi/4.1.1
      intel-oneapi-compilers/2021.4.0
      intel-oneapi-compilers/2021.4.0  intel-oneapi-mpi/2021.4.0
      intel-oneapi-compilers/2021.4.0  openmpi/4.1.1
      intel/2018.5.274
      nvhpc/21.5
      nvhpc/21.5-nompi
      nvhpc/21.7
```

Module Show command

- Format **module show <module-name>/<version>**
- Shows you the content of the module file (lua)
- This is useful if there is information on running the program included in the module
- Only works if module is available, i.e., you have modules that it depends on loaded

```
[class99@linuxclass:~]$ module show matlab/R2023b
-------------------------------------------------------------------
   /uufs/chpc.utah.edu/sys/modulefiles/CHPC-r8/Core/matlab/R2023b.lua:
-------------------------------------------------------------------
help([[This module sets the variables for Matlab R2023b
]])
setenv("MATLAB_ROOT","/uufs/chpc.utah.edu/sys/installdir/matlab/R2023b")
setenv("MLM_LICENSE_FILE","27000@ls1.chpc.utah.edu,27000@ls2.chpc.utah.edu,27
00@ls3.chpc.utah.edu")
prepend_path("PATH","/uufs/chpc.utah.edu/sys/installdir/matlab/R2023b/bin")
whatis("MATLAB R2023b")
whatis("http://www.mathworks.com")
whatis("Installed on 09/21/2023")
family("matlab")
```

Under the hood

- Module changes Environment Variables (system & application)

```
[class99@linuxclass:~]$ module list

Currently Loaded Modules:
  1) chpc/1.0 (S)

  Where:
   S:  Module is Sticky, requires --force to unload or purge



[class99@linuxclass:~]$ which matlab
/usr/bin/which: no matlab in (/uufs/chpc.utah.edu/sys/bin:/usr/loca
bin:/usr/local/sbin:/usr/sbin)
[class99@linuxclass:~]$ echo $PATH
/uufs/chpc.utah.edu/sys/bin:/usr/local/bin:/usr/bin:/usr/local/sbi
[class99@linuxclass:~]$ module load matlab
[class99@linuxclass:~]$ echo $PATH
/uufs/chpc.utah.edu/sys/installdir/matlab/R2023b/bin:/uufs/chpc.ut
in:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin
[class99@linuxclass:~]$ which matlab
/uufs/chpc.utah.edu/sys/installdir/matlab/R2023b/bin/matlab
[class99@linuxclass:~]$
```

One Name Rule and Module "Family"

- The One Name Rule:
  - Any named software with multiple versions, only one version loaded at a time
- We also define module "families"; can only have one module in a family loaded at a time
  - Used for compilers, mpi, python-based (eg conda), R-based, and etc
  - For example, if you have intel loaded, and load any gcc it will unload intel

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, but not always, the latest version is specified to be the default
- We may have depreciated older installations and their modules so some modules have been hidden
  - Many depreciated modules were from old OS, so some may not work on current OS
  - **module --show_hidden avail**

Rocky8 changes

- For intel compilers
  - intel-oneapi-compliers
- For intel mpi
  - intel-oneapi-mpi
- For intel mkl
  - intel-oneapi-mkl
- For netcdf
  - netcdf-c, netcdf-cxx, netcdf-fortran
- For pgi – now nvhpc
- For gcc – default version is gcc/8.5.0

Rocky8 changes

- For python
  - No /usr/bin/python, instead there is system python
    - /usr/bin/python2 (2.7.18),
    - /usr/bin/python3 (3.6.8)
    - For these we have created modules python/2.7.18 and python/3.6.8 so that these can be used with 'python'
  - CHPC installed 3.11.3 is default when using ml python
- For R
  - 4.4.0 is default
  - Can still use the containerized builds of R
    - R/4.4.0-basic
    - R/4.4.0-bioconductor
    - R/4.4.0-geospatial

Create your own module(s)

- Create a Conda environment (miniforge recommended) in your Home
- Install all libraries you would need (eg jupyter)
- Make it a Module
- Load module in Shell or OpenOnDemand
- For each project, create a dedicated conda env (and module)

https://www.chpc.utah.edu/documentation/software/python-anaconda.php

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
  - Help Desk: helpdesk@chpc.utah.edu
- We use chpc-hpc-users@lists.utah.edu for sending messages to users