Module 4: Finding, Downloading, and Applying Software on CURC Resources

Website: www.rc.colorado.edu

Documentation: https://curc.readthedocs.io

Helpdesk: rc-help@colorado.edu

Session Overview

- The Module System (Lmod)
- Virtual Environments with Anaconda
- Requesting Software Installations
- Advanced topics (if time permits)
  - Simplifying Source Installations with Spack
  - Containerization with Apptainer

The Module System

In most cases, a supercomputer has far more software installed than the average user will ever use.

- Users may need different versions of the same software, which in general cannot be installed nor used in parallel on the same system.
- The requirements for one package may adversely affect another package or even be mutually exclusive.

The Module System

- HPC centers manage this complexity with **environment module systems.**

- **CURC uses the Lmod system.**

The Module System

Setting up for today's session.

1. Log in to the CURC HPC system
2. Get on an Alpine compute node

```
$ module avail
$ acompile --help
$ acompile --time=2:00:00
$ module avail
```

Note: Login nodes do not have the full software stack!

The Module System

Live Demo: Loading and unloading software modules will set (and reset) important environment variables for you and will dynamically change the software environment on the cluster.

```
$ module purge
$ module load intel
$ module load hdf5
$ module display hdf5
$ env | grep HDF5
```

```
$ module purge
$ module load intel/2024.2.1
$ module avail
$ module load hdf5/1.14.5
$ module avail
```

The Module System

Live Demo: Useful Lmod commands

```
module spider                          # list all available modules
module avail                           # list modules available to you
module load <package/version>          # load a module into your env
module purge                           # unload all modules
module list                            # list currently loaded modules
module display <package>               # display module info/help
module spider <package>                # view info for all versions
module spider <package/version>        # view info for specific version
```

The Module System

Points to note about CURC-managed modules:

- CURC does not update system modules; we do fresh installs of new versions and change the default when that is appropriate
- Sometimes when a module is outdated or problematic we will remove it from the software stack

Take home: pay attention to what software modules you are loading, as this may be important for reproducibility!

Virtual Environments with CONDA

Conda is a package (software) management system

- Installs, runs, and updates packages *and their dependencies*
- Creates, saves, loads, and switches between virtual environments
- Created for Python programs, but can package and distribute software for any language

Note: Mamba is a fast, robust, and more reliable cross-platform package manager that aims to be a drop-in replacement for *Conda*

Virtual Environments with CONDA

For our system, there exists a .condarc file in your home directory

- Prevents package installs from going to your home directory

```
$ cd ~
$ cat .condarc
pkgs_dirs:
 - /projects/$USER/.conda_pkgs
envs_dirs:
 - /projects/$USER/software/anaconda/envs
```

Virtual Environments with CONDA

Environments are created and programs are installed in a few simple steps

```
$ module load anaconda
$ conda create -n my_first_env python==3.10
$ conda activate my_first_env
$ python
```

Warning: Don’t install packages in your base environment!

Virtual Environments with CONDA

Packages are installed within **activated** environments

- using conda install (preferred method, when available)
- using pip install (if you must)

```
$ conda install pandas           #install latest pandas
$ conda install pandas==0.20.3   #install specific version of pandas
```

```
$ pip install --no-cache-dir pandas       #install latest pandas
```

Warning: --no-cache-dir is crucial on CURC systems!

Virtual Environments with CONDA

Some useful conda commands

```
conda env list                          # list all environments
conda list                              # list packages in active env
conda env remove -n <envname>           # remove an environment
conda config --show channels            # view configured channels
conda deactivate                        # deactivate environment
conda create --name <clonedenv> /       # clone an environment
      --clone <envtoclone>
```

Virtual Environments with CONDA

Useful conda file paths

```
# location of python libraries
/projects/$USER/software/<env>/lib/python3.10/site-packages

# location of package executables
/projects/$USER/software/<env>/bin

# location of .condarc file
/home/$USER/.condarc
```

Want to go the extra mile?

Try our Hands-on exercise provided in EXERCISES.md. This is not required for the micro-credential.

Objectives:

1. Configure your .condarc file
2. Create a conda environment and install samtools
3. Activate the environment and run samtools.

Estimated time to complete: 15 minutes

Documentation:

https://curc.readthedocs.io/en/latest/software/python.html

Requesting Software Installations

- Is the software already installed on the cluster? https://curc.readthedocs.io/en/latest/clusters/alpine/software.html
- Have you considered its utility and complexity?
  - Are you the only user of this software?
  - How complex or difficult is this software to install?
- Have you tried installing the package on your own?
- Software request form: https://www.colorado.edu/rc/userservices/software-request

Advanced Topics

Simplifying Installations with  Spack

How can we simplify source installations?

- **Package Managers** – Tools that automate installing, maintaining, and configuring software and any dependencies
- **Environments** – A collection of resources that are available in a self-contained 'bubble'

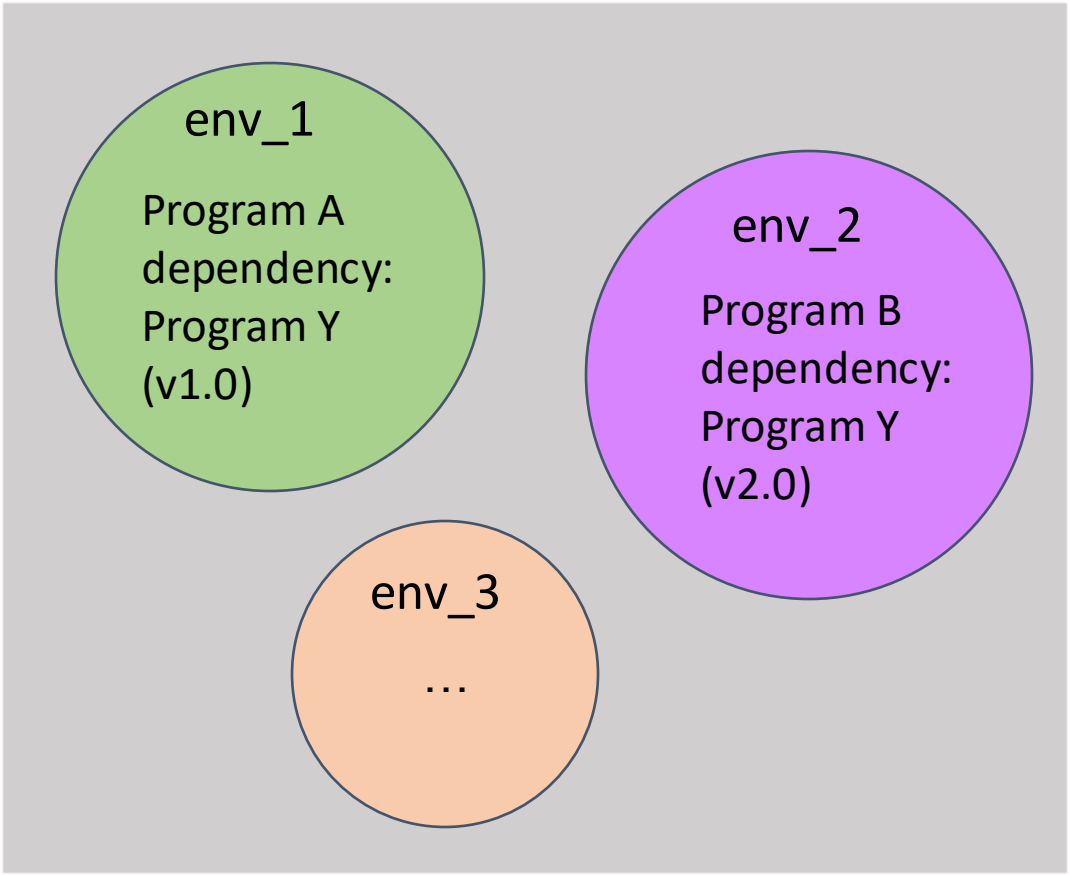
Simplifying Installations with Spack

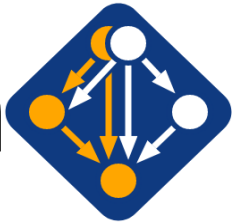
Think of virtual environments as self-contained bubbles.

env_1 contains all the dependencies of ‘Program A’.

env_2 contains all the dependencies of ‘Program B’.

The environments do not interact.

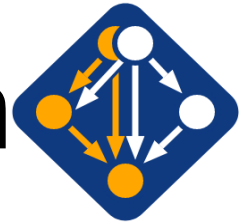


Simplifying Installations with  Spack

Environments are created and programs are installed in a few simple steps

```
$ module purge
$ module load spack/0.20.1
$ spack env create my_first_env
$ spacktivate my_first_env
$ spack install --add samtools
```

Warning: Don’t install packages outside of an environment!

Simplifying Installations with  Spack

Packages are installed within **activated** environments using spack install

```
$ spack install --add samtools      #install default samtools
$ spack install --add samtools@1.9  #install specific version
```

Simplifying Installations with  Spack

- Spack installations can be slow but will progress more quickly with more cores.
    - Spack builds all packages in parallel.
    - The default parallelism is equal to the number of cores available to the process, up to 16.

Simplifying Installations with  Spack

- Useful spack commands

```
spack env list                      # list all your environments
spack remove <env>                  # remove an environment
spack uninstall <packagename>       # remove package
spack env status                    # check which env you're in
spack info <packagename>            # prints detailed package info
spack find                          # show installed packages
despacktivate                       # deactivate environment
spack spec <packagename>            # list packages plan
```

Simplifying Installations with  Spack

- Useful spack file paths

```
# root of the spack install tree
/projects/$USER/software/spack


# location of package executables - these are symbolically linked to
      the installation tree subdirectory
/projects/$USER/spack/environments/<env>/.spack-env/view/bin


# location of spack config file
/home/$USER/.spack/config.yaml
```

Want to go the extra mile?

Try our Hands-on exercise provided in EXERCISES.md. This is not required for the micro-credential.

Objectives:

1. Create a Spack environment
2. Install fastqc in your Spack environment

Estimated time to complete: 20 minutes

Documentation:

https://curc.readthedocs.io/en/latest/software/spack.html

Containerization with  APPTAINER

Containers are portable virtualizations of an operating system, software, libraries, data, and/or workflows

- Pros
  - Portability- they can run on any system equipped with its specified container manager
  - Reproducibility- they are instances of prebuilt isolated software; the software will always execute the same every time
- Cons
  - Steeper learning curve than conda
  - Can be difficult to troubleshoot issues
  - Building containers can be tricky for multi-node MPI applications

Containerization with  APPTAINER

- CURC offers Apptainer (formerly Singularity) as container management software
  - Apptainer comes pre-installed on all Alpine nodes, so no need to load any specific software modules!
- Many common research applications have already been containerized and can be pulled from container repositories (such as Docker Hub).

Containerization with APPTAINER

Useful Apptainer commands:

```
apptainer exec          #Execute a command to your container
apptainer run           #Run your image as an executable
apptainer build         #Build a container
apptainer pull          #pull an image from hub
apptainer inspect       #See labels/environment vars, run scripts
apptainer shell         #Access the command line of your container
```

Containerization with APPTAINER

A container has its own file system and so needs help “seeing” files outside the container (on the host system). If not done in the .def file, this can be accomplished at runtime with bind mounting.

```
# bind mount a directory
apptainer run -B /source/directory:/target/directory sample-image.sif
```

On CURC systems, a running container automatically bind mounts these paths: /home/$USER, $PWD. *Note that other locations will need to be manually mounted.*

Want to go the extra mile?

- Try our Hands-on exercise provided in EXERCISES.md. This is not required for the micro-credential.

Objectives:

1. Become familiar with basic Apptainer commands.
2. Pull an image from a pre-built container, then run the program from the container.

Estimated time to complete: 20 minutes

Documentation: https://curc.readthedocs.io/en/latest/software/Containerizationon.html

Any Questions