# Installing Software on Alpine

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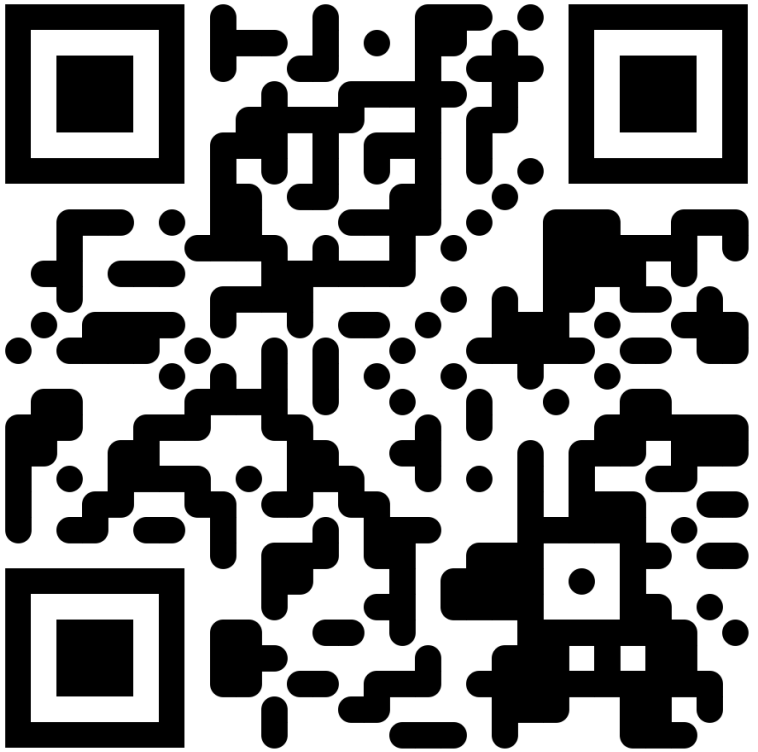
Layla Freeborn
layla.freeborn@colorado.edu

Trevor Hall
trevor.hall@colorado.edu

Research Computing
UNIVERSITY OF COLORADO BOULDER

## Slides & Exercises

https://github.com/ResearchComputing/research-software-curc



# Learning Objectives

- Learn about the different methods to install and use software on Alpine
- Gain hands-on experience with each method

# Session Overview

The Module System (Lmod)
- Setting up for today's session
- Live Demos: lmod module system

Building Software on CURC Systems
- Exercise #1: Building Software from Source

Simplifying Source installations with Spack
- Exercise #2: Building Software with Spack

Virtual Environments With Anaconda
- Exercise #3: Installing Software with Conda

Containerization With Apptainer
- Exercise #4: Installing Software With Apptainer

Requesting Software Installations

# 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.

log in to CURC

```
$ ssh <username>@login.rc.colorado.edu
```

get on an Alpine compute node

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

Research applications are not available on CURC systems from login nodes!

# The Module System


*Live Demo*: Loading and unloading modules will dynamically change the software environment on the cluster.

```
$ module load intel/2022.1.2
$ module avail
$ module load impi
$ module avail
```

```
$ module load gcc
$ module avail
$ module load openmpi
$ module avail
```

# The Module System


*Live Demo*: Loading and unloading modules will set (and reset) important environment variables for you.

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

```
$ module load gcc
$ module load hdf5
$ module display hdf5
$ env | grep HDF5
```

# 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 version
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
- Blanca modules ≠ Alpine modules
- Sometimes when a module is outdated or problematic we will remove it from the software stack

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

# The Module System

Hands-on exercise #1

**Objectives:**

1) Log in to the CU Research Computing System
2) Explore the CURC module stack

**Estimated time to complete**: 5 minutes

# Building Software on CURC Systems

- Definitions
  - **Building-** a generic term describing the overall installation process that includes compiling
  - **Compiling**- the process of converting source code to an executable
  - **Linking**- the process of combining pieces of code and data into a single file that can be loaded into memory and executed
  - **Installing**- any process that results in executables

# Building Software on CURC Systems

- There are numerous ways to install software on CURC systems
  - grab pre-compiled binaries
  - within virtual environments (using Conda, Miniconda, or Mamba)
  - using containers (Apptainer)
  - from source
  - using a package manager for HPC systems (Spack)

# Building Software on CURC Systems

Why compile a research application manually from source?

1. It is not distributed as a pre-compiled binary, by any package managers, and is not easily containerized.
2. Compiling from source on the cluster will greatly improve performance.

# Building Software on CURC Systems

Compilers are programs that convert code written in high level programming languages (like C/C++ or Fortran) to executable binary files.

# Building Software on CURC Systems

Build systems automate the process of compiling and linking.

1. GNU Build System
    - your application includes instructions to run ./bootstrap, ./autogen.sh, ./configure or make (the latter without a preceding cmake)
    - make is available in /usr/bin; Autotools available as a module

```
$ ./configure --prefix=/projects/$USER/software/bin
$ make
$ make install
```

# Building Software on CURC Systems

Build systems automate the process of compiling and linking.

2. Cmake
    - your application includes a cmake step
    - module avail cmake

```
$ cmake .. -DCMAKE_INSTALL_PREFIX=$INSTALLDIR \ --
      DCMAKE_CXX_COMPILER=g++ -DREGRESSIONTEST_DOWNLOAD=ON
$ make -j 8
$ make install
```

# Building Software on CURC Systems

Conventions and best practices

- You will need to adapt installations for **local** or **user installations** (look for these terms in the software's docs)
- Don't install software in /home/$USER (too small) or scratch (purged every 90 days); /projects/$USER/software is the way to go!
- Keep your software installations organized by using a consistent file structure and naming convention
- Load the compiler first, MPI implementation second, and third-party libraries last

# Building Software on CURC Systems

Conventions and best practices

- Don't install executables to the source directory
  - `cmake -DCMAKE_INSTALL_PREFIX, ./configure --prefix`
- The newest version of a compiler might not be compatible with your application. Read the package documentation and don't be afraid to try different compilers and compiler versions
- Read our 'Compiling and Linking' documentation https://curc.readthedocs.io/en/latest/compute/compiling.html

# Building Software on CURC Systems

Conventions and best practices

- Make life easier for yourself by adding executables to PATH and any directories with libraries that your application links to LD_LIBRARY_PATH

```
$ export PATH=/projects/$USER/software/phyloflash/bin:$PATH
$ echo $PATH
$ export
      LD_LIBRARY_PATH=/curc/sw/hdf5/1.10.1/impi/17.3/intel/17.4/lib
:$LD_LIBRARY_PATH
$ echo $LD_LIBRARY_PATH
```

# Building Software on CURC Systems

Hands-on exercise #2

**Objectives:**

1) Explore CURC compilers and compiler environment variables.
2) Perform a simple source installation.

**Estimated time to complete**: 15 minutes

# 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'

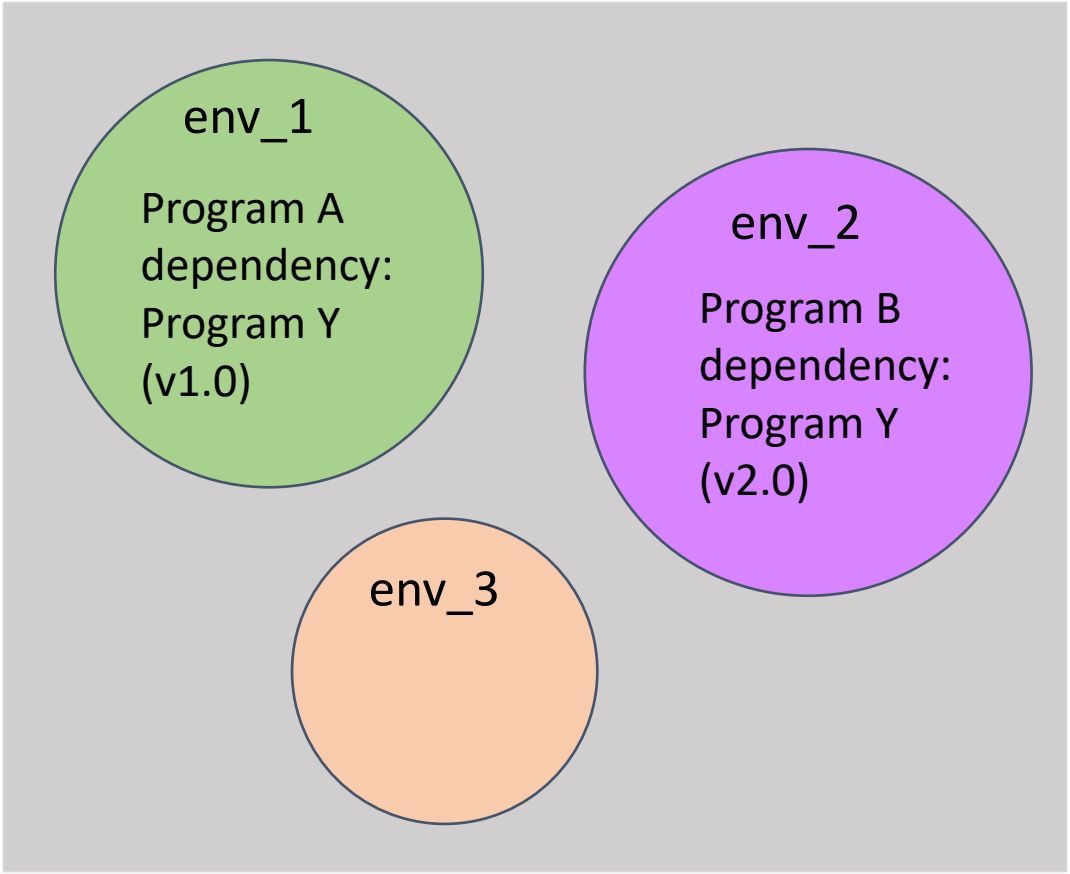
# Simplifying Installations with Spack

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

Your workflow requires two programs, ‘Program A’ and ‘Program B’.

- ‘Program A’ depends on ‘Program Y’ **v1.0**
- ‘Program B’ depends on ‘Program Y’ **v2.0**

What do you do?!

# Simplifying Installations with  Spack

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

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

*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
```

# Simplifying Installations with  Spack

Hands-on exercise #3

**Objectives:**
1) Create a Spack environment
2) Install fastqc in your Spack environment

**Estimated time to complete**: 20 minutes

# 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

# 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
```

*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)

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

# Virtual Environments With CONDA

- Packages are installed within **activated** environments

using **pip install** (if you must)

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

*--no-cache-dir is crucial on CURC systems!*

# Virtual Environments With CONDA

- 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
```

# Virtual Environments With CONDA

Hands-on exercise #4

**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

# Containerization With  APPTAINER

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

- pros
  - portability- containers can run on any system equipped with its specified container manager
  - reproducibility- because containers 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

Many common research applications have already been containerized and can be pulled from container repositories.

- Use prebuild containers when you can!
- Email rc-help@colorado.edu if you want to build custom containers

# Containerization With APPTAINER

## Useful singularity 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         #Shell into your image
```

# 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.*

# Containerization With  APPTAINER

Hands-on exercise #5

**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

# 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

# Thank you!