Research Software on CURC Systems

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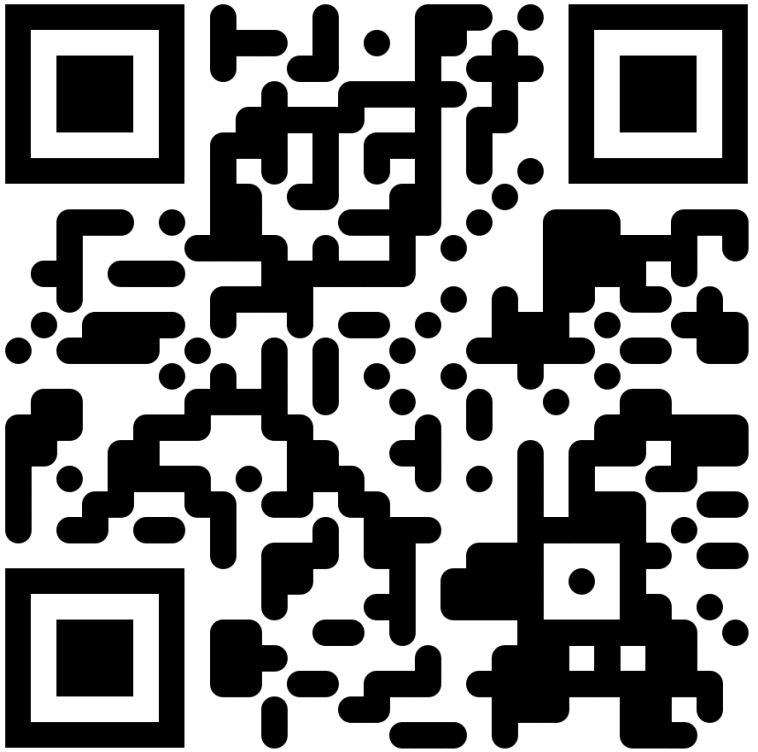
Slides & Exercises

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



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 (Singularity)

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 lafr9499@login.rc.colorado.edu
```

get on an Alpine compute node

```
1  module avail
2  acompile --help
3  acompile --time=90:00
4  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.

```
1  module load intel/2022.1.2
2  module avail
3  module load impi
4  module avail
```

```
1  module load gcc
2  module avail
3  module load openmpi
4  module avail
```

The Module System

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

```
1  module load intel
2  module load hdf5
3  module display hdf5
4  env | grep HDF5
```

```
1  module load gcc
2  module load hdf5
3  module display hdf5
4  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 ≠ Summit 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!

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/Singularity)
  - 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

```
1  ./configure --prefix=/projects/$USER/software/bin
2  make
3  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`

```
1  cmake .. -DCMAKE_INSTALL_PREFIX=$INSTALLDIR \
       --DCMAKE_CXX_COMPILER=g++ -DREGRESSIONTEST_DOWNLOAD=ON
2  make -j 8
3  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

```
1  export PATH=/projects/$USER/software/phyloflash/bin:$PATH
2  echo $PATH
3  export
   LD_LIBRARY_PATH=/curc/sw/hdf5/1.10.1/impi/17.3/intel/17.4/lib:$L
   D_LIBRARY_PATH
4  echo $LD_LIBRARY_PATH
```

Building Software on CURC Systems

Hands-on exercise #1.

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'

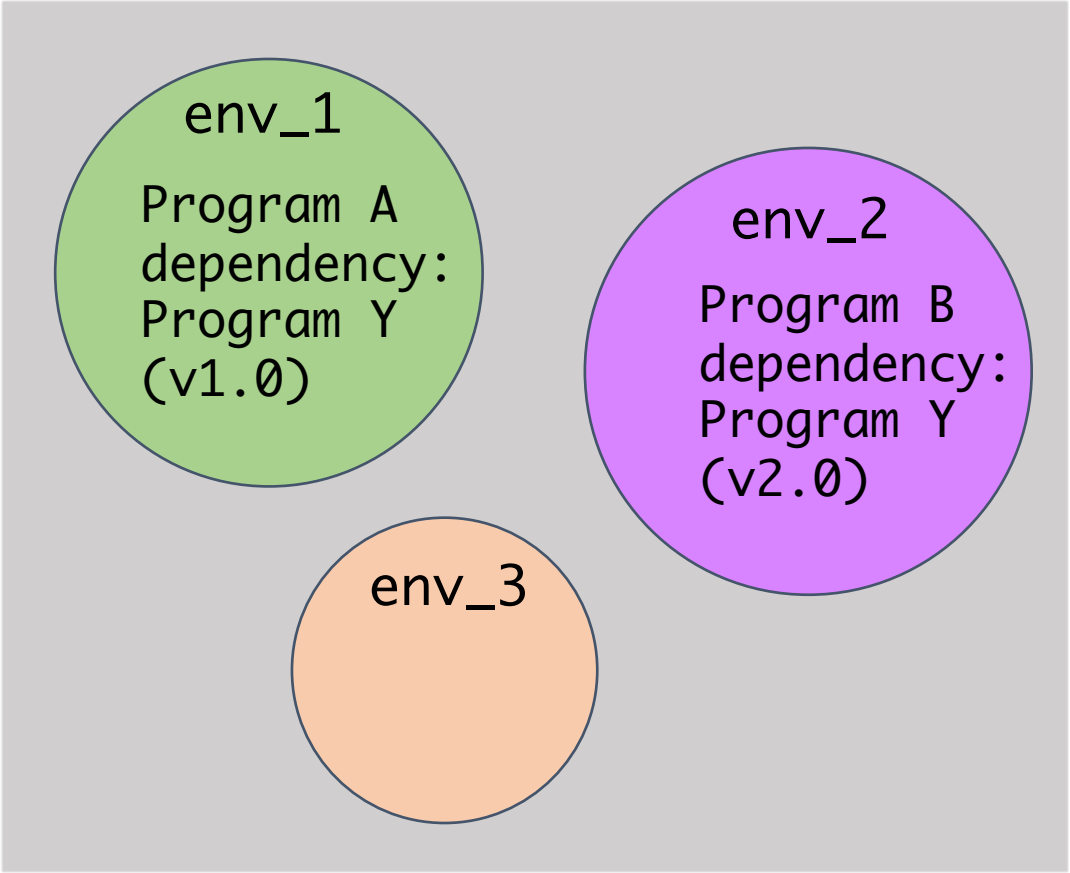
Simplifying Installations with Spack

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

```
1    module load spack/0.20.1
2    spack env create my_first_env
3    spacktivate my_first_env
4    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 of
                                       samtools
```

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 #2.

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

```
1    module load anaconda
2    conda create -n my_first_env python==3.10
3    conda activate my_first_env
4    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 #3.

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 (Singularity) as container management software

- `module load singularity`

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

`singularity` commands can generate large temporary and cache files. To manage this, export the following environment variables prior to running `singularity`.

```
# set cache directory to Alpine scratch
export SINGULARITY_CACHEDIR=/scratch/alpine/$USER
# set tmp directory to Alpine scratch
export SINGULARITY_TMPDIR=/scratch/alpine/$USER
```

Containerization With  APPTAINER

Useful `singularity` commands

```
singularity --help                              # view help for all singularity commands
singularity pull                                # download or build a container from a
                                                  registry
singularity inspect --deffile <name.sif>        # inspect the container definition file
singularity run <name.sif>                      # run container with default commands
                                                  (not always available)
singularity exec <name.sif> <command>           # run a specific command that is defined
                                                  within the container
singularity shell <name.sif>                    # run a shell within the 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
singularity run -B /source/directory:/target/directory sample-image.sif
```

On CURC systems, a running container automatically bind mounts these paths: `/home/$USER`,`/projects/$USER`, `/scratch/alpine/$USER`,`/rc_scratch/$USER`,`/tmp`, and the directory from which the container was run.

Containerization With  APPTAINER

Hands-on exercise #4.

Objectives:

1) Become familiar with basic Singularity commands.

2) Pull an image from a pre-built container, then run the program from the container.

Estimated time to complete: 15 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!