Installing and Using Software on CARC Systems

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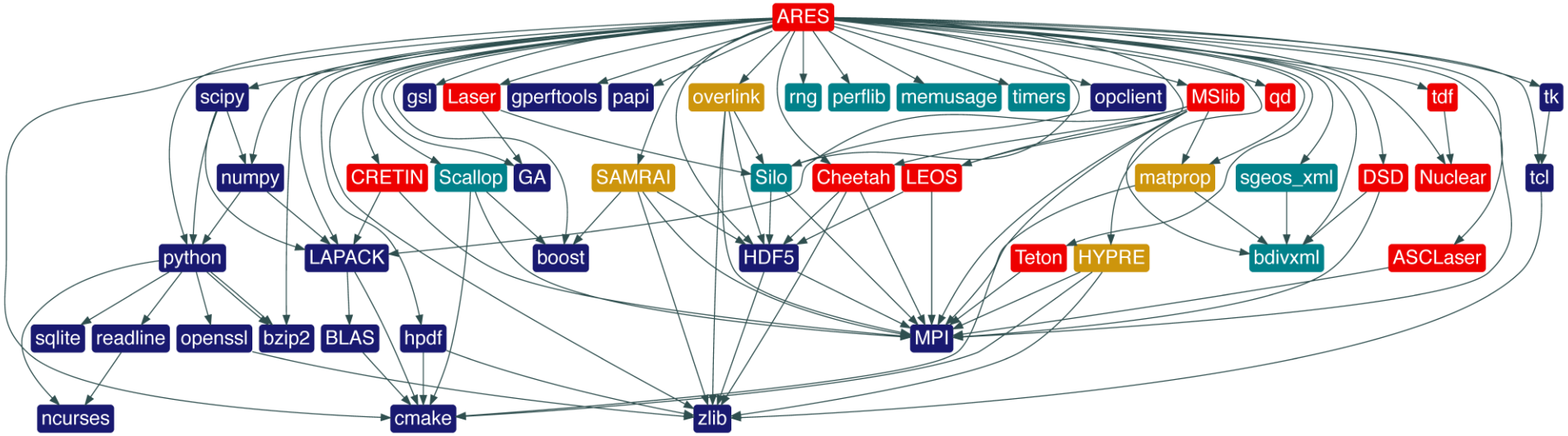
Outline

- CARC managed software
  - Finding software
  - Using modules
  - Neat features
- Installing software
  - Precompiled binary
  - Conda
  - Python
  - R
  - Singularity
  - Building Source Code

Software is complex!

- Dependency graph for ARES



https://computing.llnl.gov/projects/spack-hpc-package-manager

What are software modules?

- Modules present installed software to users
- Set environment variables
  - PATH
  - PKG_CONFIG_PATH
  - LD_LIBRARY_PATH
  - <SOFTWARE>_ROOT
- Show how package was built
- Show where package was installed to
- Prevent loading incompatible software
- Writen in Lua

What are software modules?

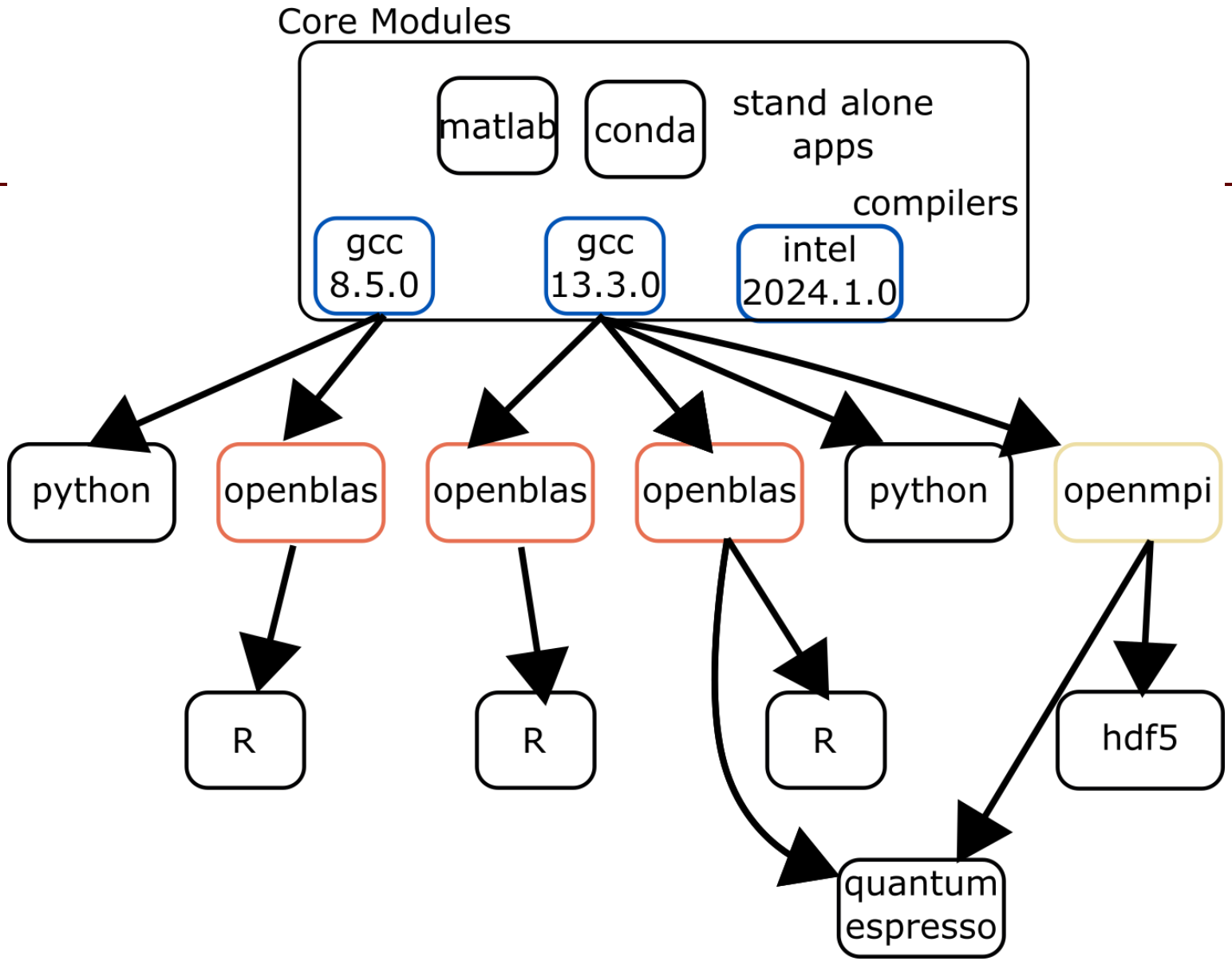
- There are 4 kinds of modules
  - Utilities
    - git, screen, tmux, wget, ...
  - Compiler (gcc, intel)
  - BLAS
    - openblas, mkl, amd-blis
    - Math Library
  - MPI
    - OpenMPI, mvapich2, IntelMPI
    - Multi node communication
  - Application
    - most common, bamtools, cmake, libpng...
  - Other
    - Matlab, Mathematica, julia,

What are software modules?

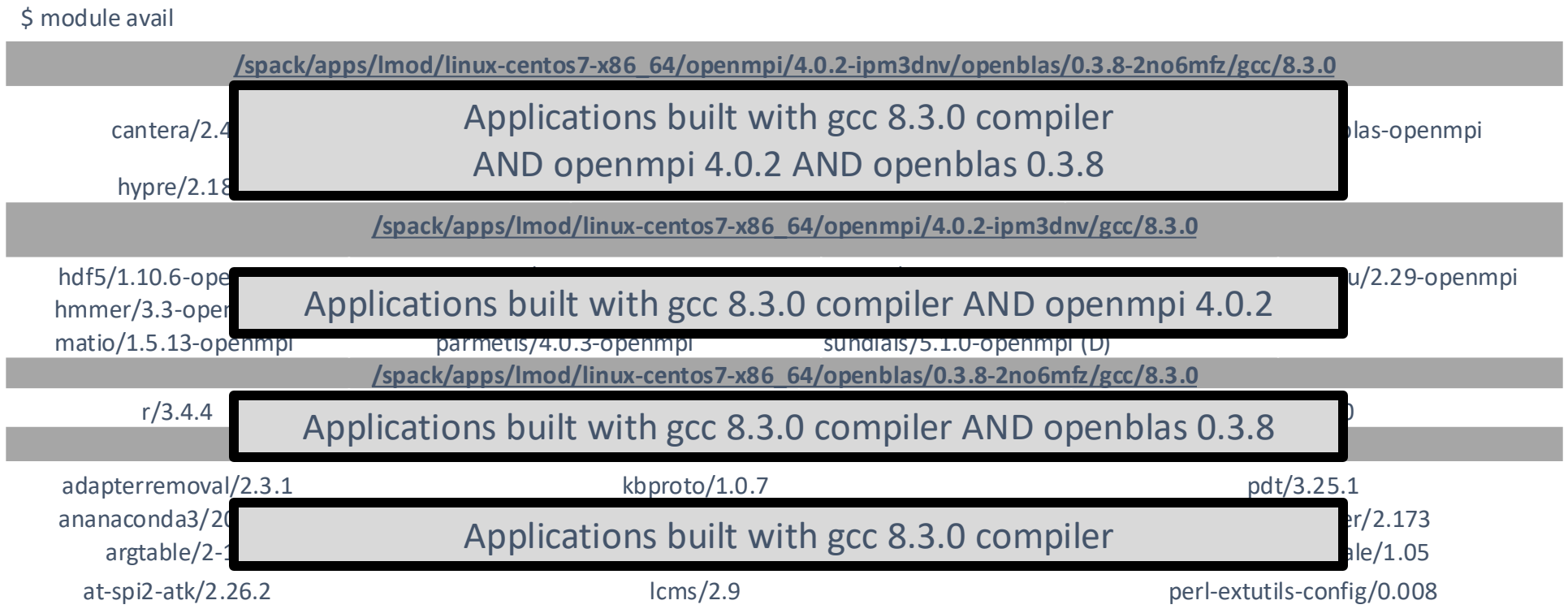
- By default you have the recommended "usc" module loaded

```
$ module list
Currently Loaded Modules:
  1) gcc/13.3.0       3) openblas/0.3.28   5) usc/13.3.0
  2) python/3.11.9    4) openmpi/5.0.5
```

- You can check what's available with module avail
- Depending on active modules, you will see different results from `module avail`


Core Modules
matlab
conda
stand alone apps
compilers
gcc 8.5.0
gcc 13.3.0
intel 2024.1.0
python
openblas
openblas
openblas
python
openmpi
R
R
R
hdf5
quantum espresso

Example module avail listing



How to use modules

- Use module avail to see what's available
- Use module load to load the module

```
$ which python
/usr/bin/python

$ module load python

$ which python
/apps/spack/2406/apps/linux-rocky8-x86_64_v3/gcc-
13.3.0/python-3.11.9-x74mtjf/bin/python
```

- Some modules 'unlock' more modules
  - Compiler
  - MPI
  - BLAS

Finding modules

- Use module spider to search for software that's not available
  - Might be hidden due to prerequisites

```
$ module spider r/4.4.2

----------------------------------------------------
  r: r/4.4.2
----------------------------------------------------


    You will need to load all module(s) on any one of the lines below before the "r/4.4.2" module is
available to load.


     gcc/13.3.0
```

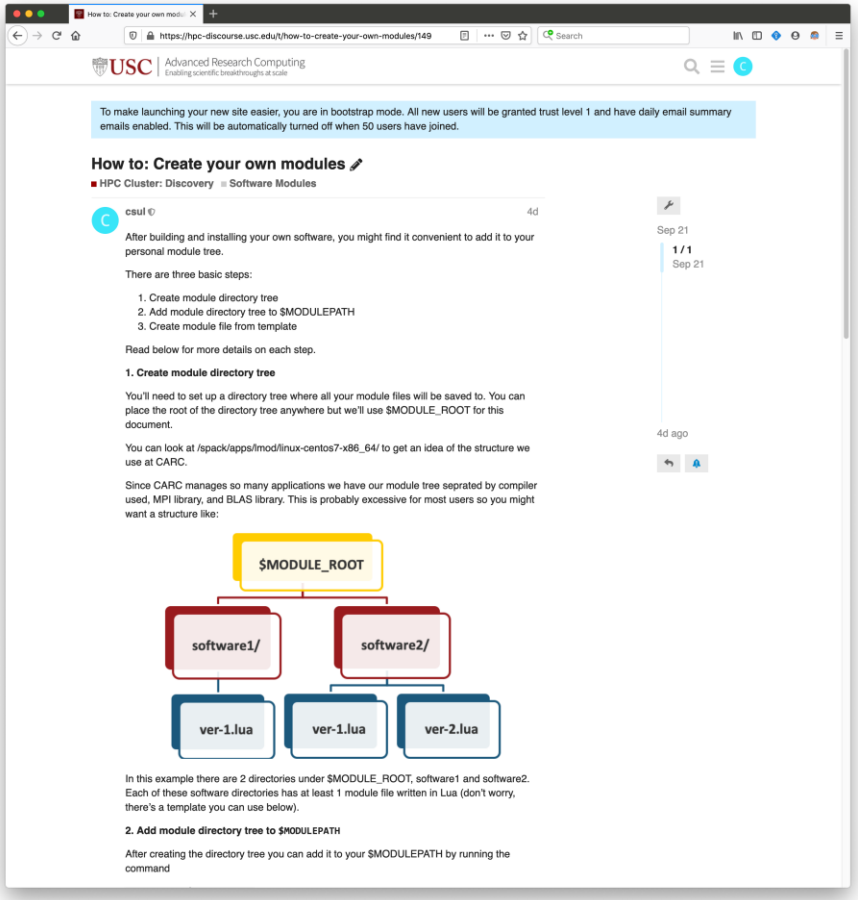
Saving sets of modules

- If you find yourself loading a set of modules frequently

`module save`	Save current modules to default collection
`module save <name>`	Save current modules as `<name>` collection
`module restore`	Load modules in default collection
`module restore <name>`	Load modules in `<name>` collection
`module describe <name>`	Show which modules are in `<name>` collection
`module savelist`	Show names of all collections

Creating your own modules

- Check our Discourse page for more details
- [How to: Create our own modules]



Installing Your Own Software

Installing software

- Installing software can be quick and painless
  - With precompiled binaries for your specific operating system, it can be as easy as unzipping a file
- … or neither quick nor painless
  - If you have to compile the software yourself using compilers, linkers, Makefiles, external libraries, etc.
- (or even worse...)
  - If it's from an academic lab from 1999 and requires old versions of multiple libraries which have multiple dependencies!

Installing software

- Generally speaking, software can be installed globally or locally
  - On your laptop, you are the system administrator
  - On HPC, you are not the system administrator
- Globally means system-wide
  - Software is installed to system locations like /usr/bin or /usr/local
  - Global installs require root privileges
- System-wide installations will not work on HPC
  - Only systems administrators have root privileges on HPC
  - E.g., ”yum install” and “apt install” will not work

Installing software

- CARC users must perform local, or “user”, installs
  - Software installed to 'local' folders
    - /project/<pi_id>/software
  - Requires write privileges, which you have in your own directories
  - Software will be accessible by you, even on compute nodes
- It is not always obvious how to perform a user install
  - Depends on software
  - You may have to check documentation

Precompiled binary

- Simplest case
- Just download and extract
- Not always available

```
$ cd /project/ttroj_412/software

#Copy tarball
$ wget https://example.com/sample.tar.gz

#Extract files
$ tar xvf sample.tar.gz

#Set your environment (adds a new location to your path)
$ export PATH=/project/ttroj_412/software/sample/bin:${PATH}

#Test installation
$ binary_name
```

Conda Environments

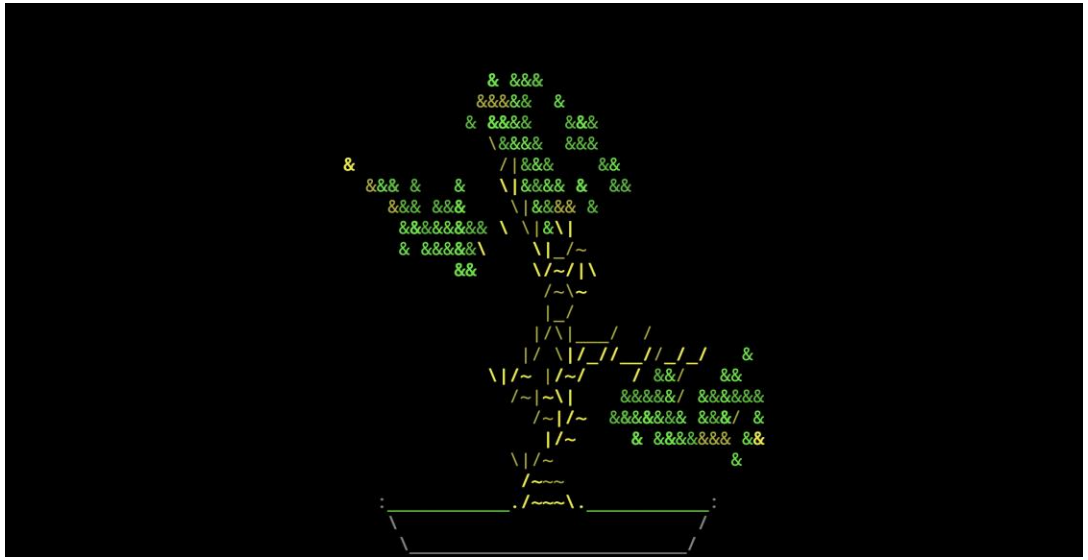
Conda Environments

- Some developers package their software as conda environments
- Create a collection of software packages
- Dependencies are managed for you
- mamba env create -f envrionment.yml
- Full documentation here

```
name: mustache
channels:
  - conda-forge
  - defaults
dependencies:
  - pip
  - h5py
  - hdf5
  - numpy
  - python=3.8
  - pip:
    - cooler
    - hic-straw
    - pandas
    - scipy
    - statsmodels
```

Our own environment

- We can also create our own custom environments
- Let's use "cbonsai" example
- Prints ascii art of bonsai tree



Our own environment

- Set up conda

```
$ module load conda

$ mamba init bash
```

- Create and name environment

```
$ mamba create -n cbonsai
# Enter environment
$ mamba activate cbonsai
```

- Install packages

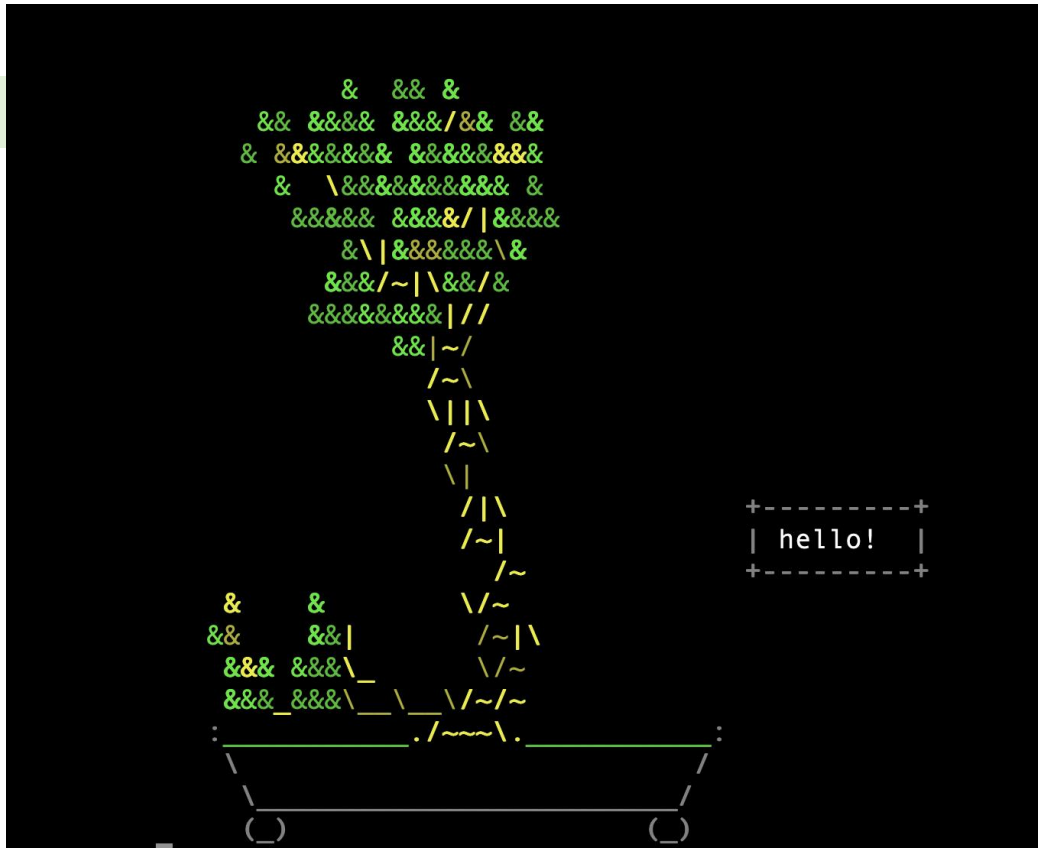
```
$ mamba install cbonsai
```

```
$ mamba install cbonsai
.
.
.
  Package         Version  Build       Channel         Size
──────────────────────────────────────────────────────────────
  Install:
──────────────────────────────────────────────────────────────


  + _libgcc_mutex     0.1  conda_forge  conda-forge      3kB
  + libgomp        14.2.0  h77fa898_1   conda-forge    461kB
  + _openmp_mutex     4.5  2_gnu        conda-forge     24kB
  + libgcc         14.2.0  h77fa898_1   conda-forge    849kB
  + ncurses           6.5  h2d0b736_3   conda-forge    892kB
  + cbonsai        1.3.1  haa1a288_0   conda-forge     30kB


  Summary:


  Install: 6 packages


  Total download: 2MB
```

Our own environment

- Run cbonsai

```
$ cbonsai -m hello! -p
```



Installing Python Packages

Installing Python packages

- Don't forget to load the version of python you want to use

```
$ module load python/3.7.6
```

- To check what packages are available use the command

```
$ pip list
```

- Install package (bash shell)

```
$ pip install <package_name> --user
```

- Sometimes you'll need to install the latest version of a package that is already installed

```
$ pip freeze
$ pip install <package_name> --upgrade --user
```

Dependencies for Python packages

- Some packages are Python wrappers for C/C++ libraries
- The installer needs to know where these libraries are
- The h5py package is one example

```
$ HDF5_DIR=/path/to/hdf5
$ HDF5_VERSION=X.Y.Z
$ CC="mpicc"
$ pip install h5py --user
```

- You might have to download the package tarball and edit some files like setup.py

Installing R Packages

Installing R packags

- Source the version of R you want to use and start R

```
$ module load r
$ R
```

- Install package syntax (you may have to specify a path)

```
> install.packages('<package_name>')
> install.packages('<package_name>", lib="/path/to/packages")
```

- Then load the library when you want to use

```
> library('<package_name>’)
> library('<package_name>’, lib.loc="/path/to/packages")
```

Dependencies for R packages

- Some packages are R wrappers for C/C++ libraries
  - The installer needs to know where these libraries are
  - You might have to download the package tarball and edit some files
- You can set compilation environment variables like LDFLAGS in the file ${HOME}/.R/Makevars

Singularity/Containers

Apptainer

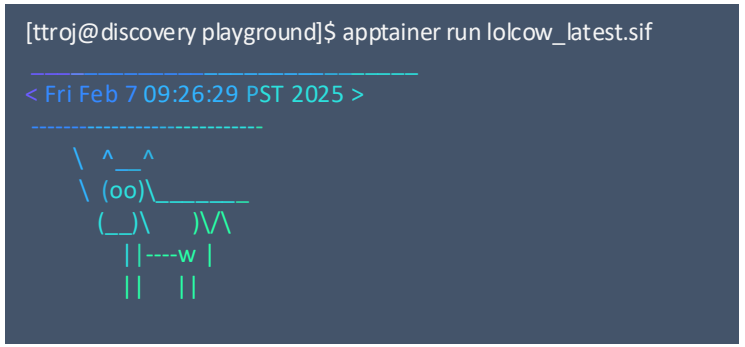
- Formerly Singularity
- For difficult installations
- Apptainer provides packaged "computing environments"
- Works best with complex dependency chains
- Compatible with Docker

Apptainer

Example: lolcow (date|cowsay|lolcat)

```
#Download container image
$ apptainer pull docker://ghcr.io/apptainer/lolcow

#Test
$ singularity run lolcow_latest.sif
```

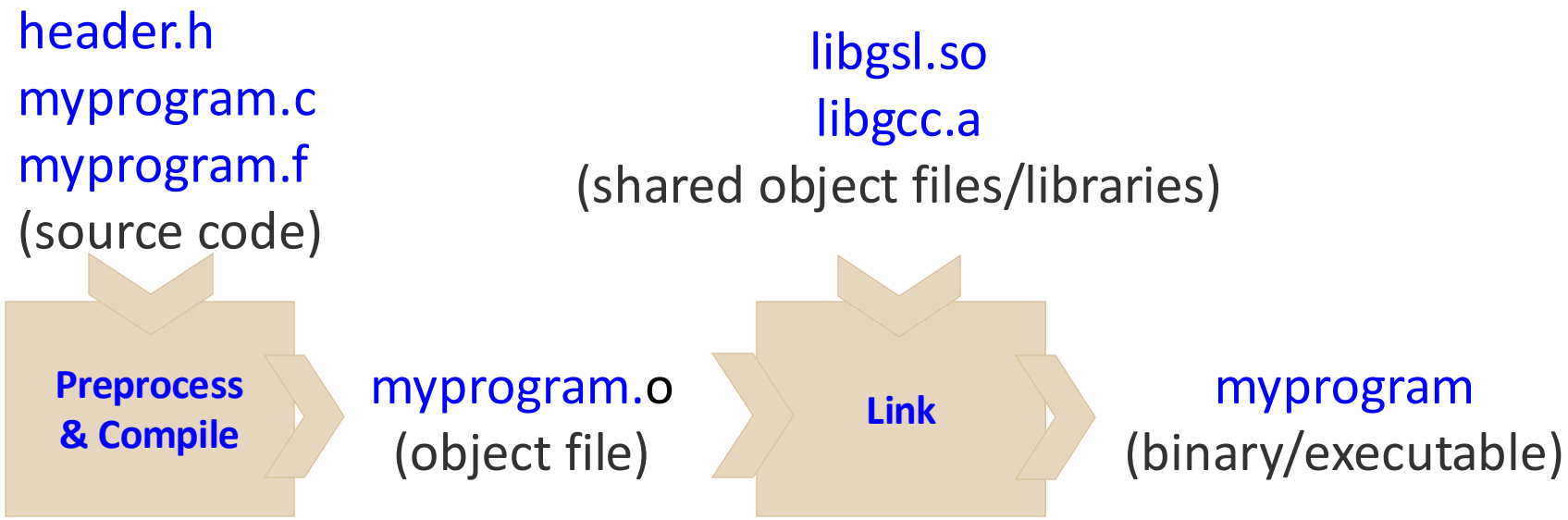
See this page for more ways to interact with a container:
https://apptainer.org/docs/user/latest/quick_start.html#interacting-with-images



Building Source Code

Compiling to source code

- C/C++ and Fortran programs are compiled and assembled



Compilers

- A typical compile command for C code

```
$ gcc ${CCFLAGS} source.c ${CPPFLAGS} ${LDFLAGS} –o myprogram
```

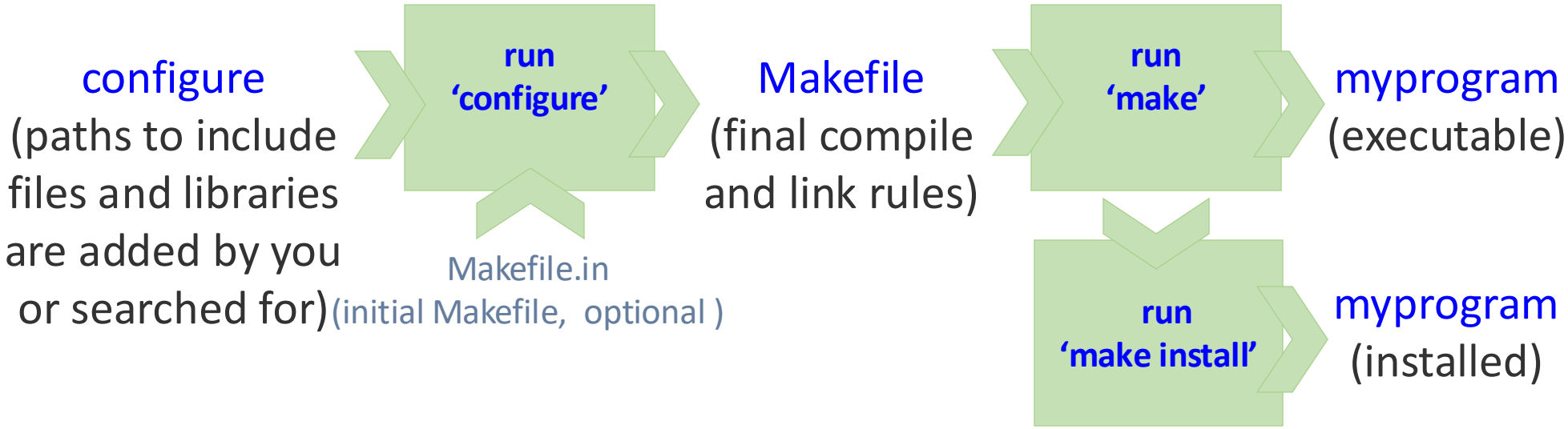
- Where these environment variables were pre-defined

```
$ CCFLAGS='-Wall -O3'
$ CPPFLAGS='-I/path/to/include'
$ LDFLAGS='-L/path/to/lib -lgsl -lgslcblas –lm’
```

CCFLAGS	Flags to pass the C compiler
CPPFLAGS	Where the C preprocessor can find include (.h) files
LDFLAGS	Which libraries (.so, .a files) to use and where the linker can find them

With configure/make

- Manually typing compile and link commands is not feasible
- Software build utilities like autotools, cmake handle this



Building software with modules

- Most modules modify `$PKG_CONFIG_PATH`
- Many installer scripts check here for prerequisite software

```
$ module load ncurses
$ ./configure <options>
...
checking curses.h usability... yes
checking curses.h presence... yes
checking for curses.h... yes
checking ncurses.h usability... yes
checking ncurses.h presence... yes
checking for ncurses.h... yes
...
```

- If we're lucky it's that easy

Building software with modules

- If unlucky, specify with script options

```
module load ncurses
./configure --ncurses-root=${NCURSES_ROOT} <other options>
...
checking curses.h usability... yes
checking curses.h presence... yes
checking for curses.h... yes
checking ncurses.h usability... yes
checking ncurses.h presence... yes
checking for ncurses.h... yes
...
```

- Our modules set environment variable `<software>_ROOT` for just this occasion

Building software with modules

- If very unlucky, modify Makefile

```
...
override LDFLAGS += -L./nicksrc -L$(GSL_ROOT)/lib
-L$(OPENBLAS_ROOT)/lib

override CFLAGS += -c -g -p -Wimplicit -I./ -I./nicksrc
-I$(GSL_ROOT)/include -I$(OPENBLAS_ROOT)/include
...

$ module load ncurses
$ make
```

Compiling source code

Example: vim

```
#Download tarball
$ git clone https://github.com/vim/vim.git
$ cd vim

#Run configure script
$ ./bootstrap
$ ./configure --prefix=/project/<pi_id>/<username>/vim [other options]

#Run makefile
$ make
$ make install
```

Compiling source code

- Configure script can't find libtinfo.so (provided by ncurses)

```
checking --with-tlib argument... empty: automatic terminal library selection
checking for tgetent in -ltinfo... no
checking for tgetent in -lncurses... no
checking for tgetent in -ltermlib... no
checking for tgetent in -ltermcap... no
checking for tgetent in -lcurses... no
no terminal library found
checking for tgetent()... configure: error: NOT FOUND!
```

Compiling source code

- In this case, pkg-config is not used
- Manually override with pkg-config, $LDFLAGS, and $CPPFLAGS

```
$ pkg-config --cflags-only-I ncurses
-D_GNU_SOURCE -I/spack/apps/linux-centos7-x86_64/gcc-8.3.0/ncurses-6.1-
akiyo4qrgzlzxw3hggkc42nvv7hz2evj/include

$ pkg-config --libs-only-L ncurses
-L/spack/apps/linux-centos7-x86_64/gcc-8.3.0/ncurses-6.1-akiyo4qrgzlzxw3hggkc42nvv7hz2evj/lib
```

Compiling source code

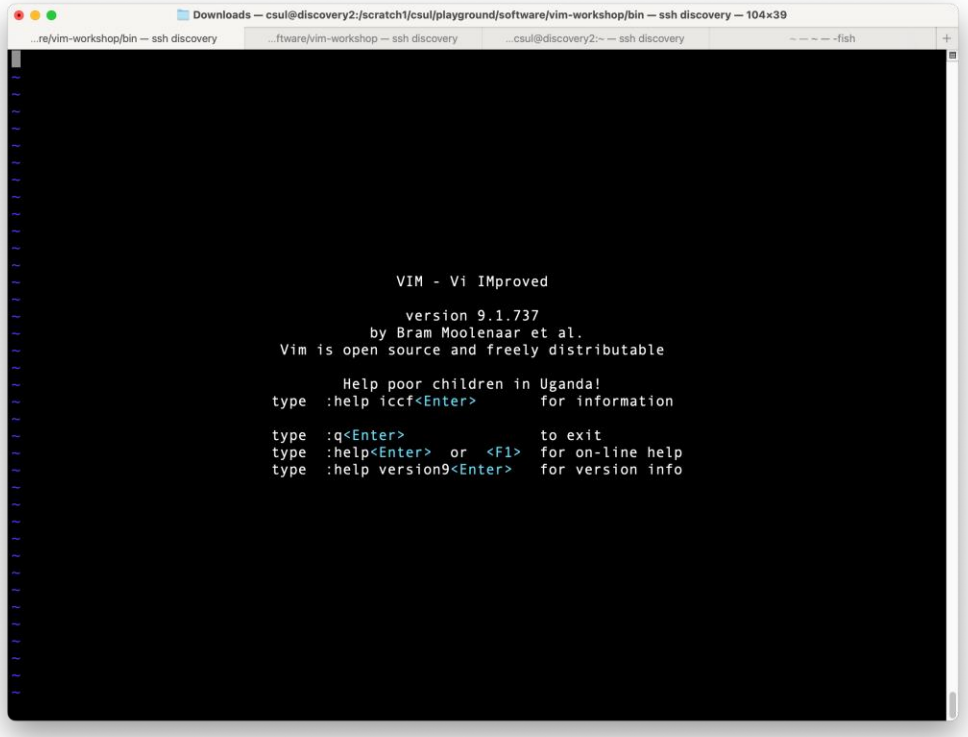
Example: vim

```
#Download tarball
$ git clone https://github.com/vim/vim.git
$ cd vim

#Run configure script
$ CPPFLAGS=$(pkg-config --cflags ncurses) \
LDFLAGS=$(pkg-config --libs-only-L ncurses) \
./configure \
--prefix=/project/<pi_id>/<username>/vim \
--with-tlib=tinfo

#Run makefile
$ make
$ make install
```

Compiling source code

Test installation

```
$ ./vim # :q! to quit
```



Getting Help

- Request assistance
  - Email carc-support@usc.edu
  - Office Hours (drop-in)
    - Every Tuesday@2:30pm (Zoom)
- Learn more!
  - Visit carc.usc.edu
  - Request a consultation (anytime)
  - Attend a Workshop (when scheduled)
  - Visit our Discourse page!

Thank you for attending!

Questions?

carc-support@USC.EDU