THE UNIVERSITY OF UTAH™

TOGETHER WE REACH

Center for High-Performance Computing

Introduction to Containers

Martin Čuma
Center for High Performance Computing
University of Utah
m.cuma@utah.edu

Overview

- Why do we want to use containers?
- Containers basics
- Run a pre-made container
- Build and deploy a container
- Containers for complex software

Hands on setup

1. Download the talk slides

   http://home.chpc.utah.edu/~mcuma/chpc/Containers24s.pdf

2. Using FastX or Putty, ssh to any CHPC Linux machine, e.g.

```
$ ssh uxxxxxx@frisco.chpc.utah.edu
```

3. Load the Apptainer module

```
$ module load apptainer
```

Why to use containers?

Software dependencies

- Some programs require complex software environments
  - OS type and versions
  - Drivers
  - Compiler type and versions
  - Software dependencies
    - glibc, stdlibc++ versions
    - Other libraries and executables
    - Python/R/MATLAB versions
    - Python/R libraries

Reproducible research

- Research outputs include software and data
- Software reproducibility
  - Software repositories (svn, git)
  - Good but often software has dependencies
- Data reproducibility
  - Data as publication supplementary info, centralized repositories (NCBI), …
  - Disconnected from the production environment
- Package data AND code AND compute environment in one file

Scalable research

- Develop a program / pipeline locally, run globally
- Scale to parallel resources
  - Run many times
  - Use local or national HPC resources
- Automate the process
  - Container/software building and deployment
  - Parallel pipeline

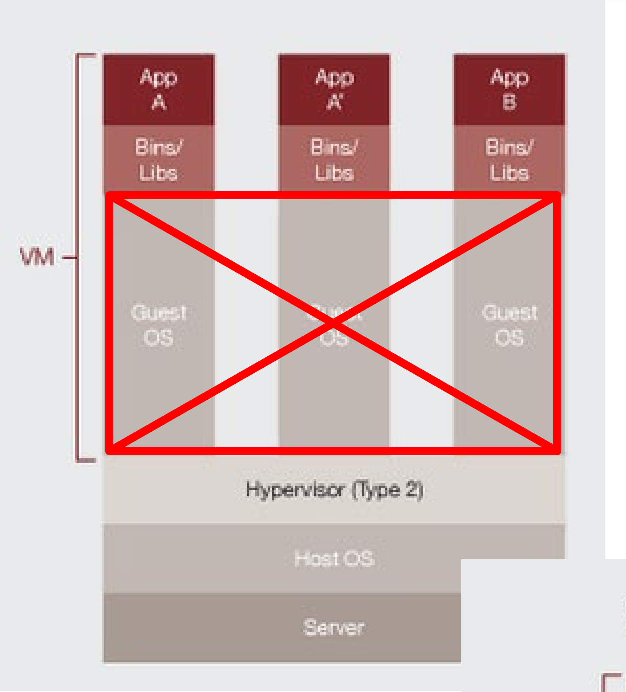
Additional bonus

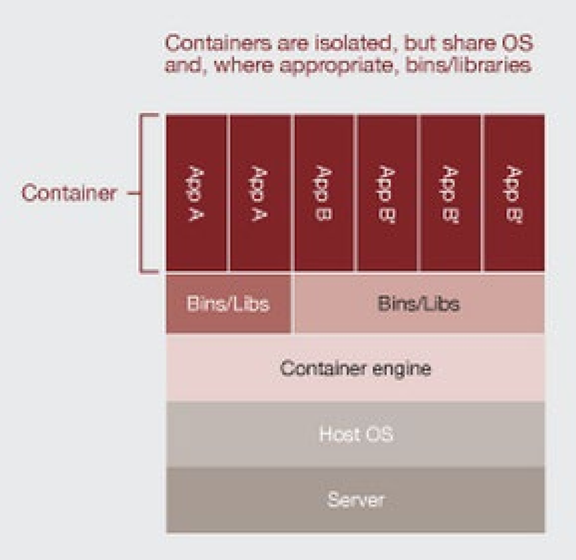
- Old applications built on old Linux versions can run on newer Linux host, and vice versa
- May be able to run Windows programs on Linux

Container basics

Virtualization basics

- Hardware virtualization
  - Running multiple OSes on the same hardware
  - VMWare, VirtualBox
- OS level virtualization
  - run isolated OS instance (guest) under a server OS (host)
  - Also called containers; user defined software stack (UDSS)
  - Docker, Singularity, Apptainer





Containers

- Isolate computing environments
  - And allow for regenerating computing environments
- Guest OS running over host OS
  - Guest's OS can be different that host's
  - Low level operations (kernel, network, I/O) run through the host
- From user standpoint guest OS behaves like standard OS

Container solutions

- Docker
  - Well established
  - Has docker hub for container sharing
  - Problematic with HPC
- Singularity, Apptainer
  - Designed for HPC, user friendly
  - Support for MPI, GPUs
- Charliecloud; Shifter, udocker
  - Also HPC designed, more Docker compatibility
  - Simple, but less practical

Container solutions - contd.

- OS vendor tools
  - RedHat Podman, Buildah, Skopeo - new with RHEL 8
- Other Linux based container solutions
  - runC, LXC
- Orchestration tools
  - use containers to spin up groups of servers
  - Kubernetes, Docker Compose

Singularity containers

- Integrate with traditional HPC
  - Same user inside and outside of the container
  - Same file systems (home, scratch), environment
  - Can integrate with existing software (CHPC sys branch)
- Portable and sharable
  - A container is a file
  - It can be built on one OS and run on another
- Only Linux support right now
- Possible security issues due to the use of setUID executables
  - Hacker can exploit potential flaws in setUID programs to gain root
  - https://sylabs.io/guides/3.8/user-guide/security.html

An aside into security

- Containers need privilege escalation to run
  – Give sudo
  – Run root owned daemon process (Docker)
  – Use setUID programs (programs which parts can run in privileged mode) (*Singularity* now, udocker)
  – User namespaces – new Linux kernel feature to further isolate users (*Apptainer*, *Charliecloud*, limited Singularity, Docker)
  – Linux capability set – fine grained privilege isolation (Singularity future?)
- In HPC environment
  – setUID if you have some trust in your users, user namepaces if you don't (and have newer Linux distribution – e.g. CentOS >= 7.4)

Singularity and Apptainer

- Singularity
  - Originally developed at LLNL
  - Spun out into a venture capital funded company to allow for growth
  - Remained open source but company interests diverged
  - Company (Sylabs) runs the Sylabs Cloud
- Apptainer
  - Forked from open source Singularity, but diverged since
  - Funded by the Linux Foundation
  - Rootless container build
  - Our future choice for now due to staying open source and active development

Charliecloud containers

- Uses user namespaces for isolation
  - More secure, rootless
  - Requires newer Linux OSes (works well on Rocky Linux 8)
- Better Docker compatibility
  - Uses Dockerfiles for build
  - Uses the same layers as Docker
  - Good option for building a container when one has a Dockerfile
  - See instructions at https://www.chpc.utah.edu/documentation/software/charliecloud.php

Singularity workflow

Interactive Development

apptainer build --sandbox tmpdir Singularity
~~sudo singularity build --sandbox tmpdir/ Singularity~~

~~sudo singularity build --writable container.img Singularity~~

Build from Recipe

apptainer build container.sif Singularity
~~sudo singularity build container.img Singularity~~

Remote build on Sylabs Cloud

~~sudo~~ singularity build --remote container.sif Singularity

Build from Docker

apptainer build container.sif docker://ubunu
~~sudo~~ singularity build container.img docker://ubuntu

BUILD ENVIRONMENT

Container Execution

singularity run container.img
singularity shell container.img
singularity exec container.img ...

Reproducible Sharing

singularity pull shub://...
singularity pull docker://... *

PRODUCTION ENVIRONMENT

* Docker construction from layers not guaranteed to replicate between pulls

Run a pre-made container

A few pre-requisites

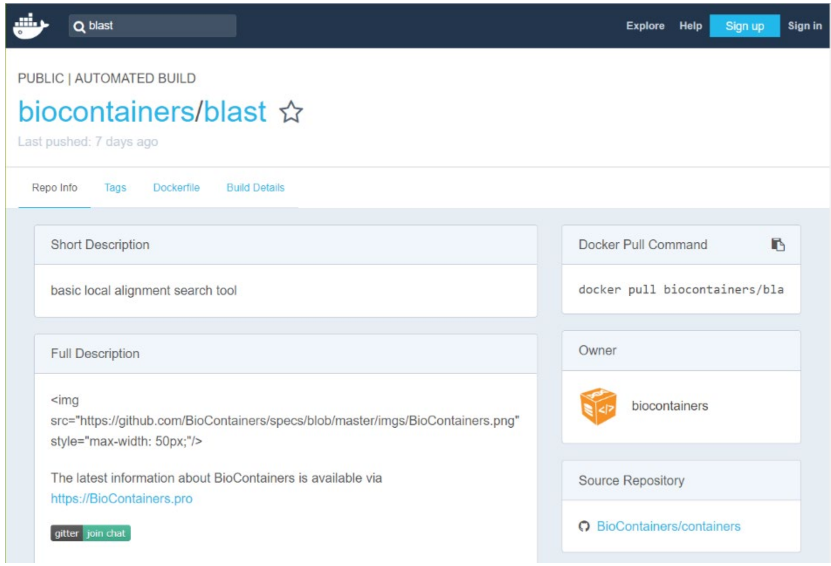
- Building a container often requires a root, or sudo
  - You can do that on your own machine
  - You can do that in the cloud (e.g. Sylabs Cloud, Docker Hub).
- Some container runtimes are rootless
  - You can build at CHPC clusters with Apptainer or Charliecloud
- You can run a container as an user
  - You can run your own containers at CHPC
  - You can run CHPC provided containers at CHPC
  - You can run containers obtained on the internet at CHPC

Basic principles

- Containers are run in user space (no root required)
- An appropriate environment module has to be loaded
  - Apptainer, Singularity, Charliecloud
- User inside of the container
  - Current user
  - If specified, other user, including root
  - Root inside container is contained = can't be root outside
- Some containers can be modified by non-root user
  - Apptainer, Charliecloud

Container registries and repositories

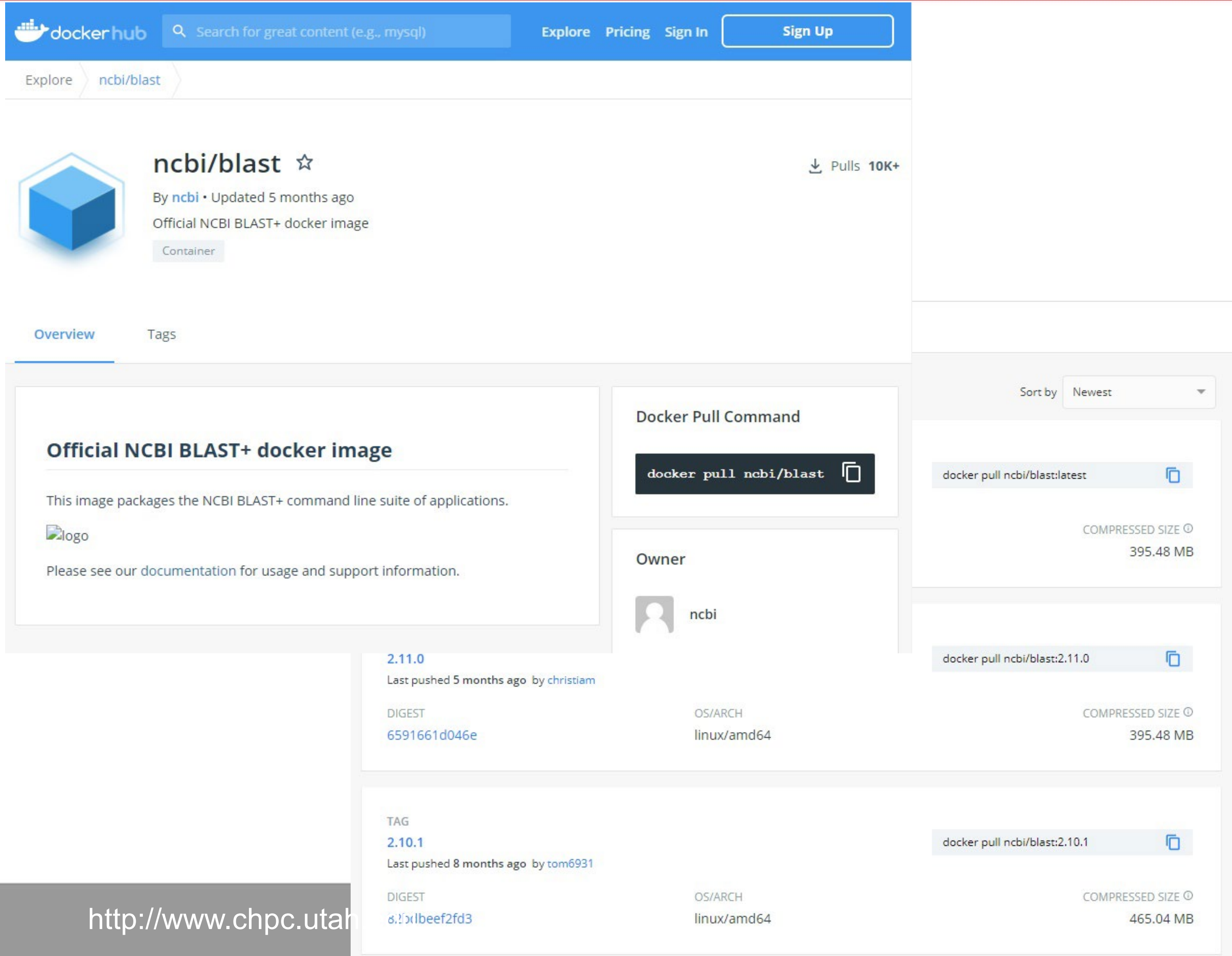
- Most containers reside in registries
  - Content delivery and storage systems for container images
- Docker Hub is the most common registry
  - https://hub.docker.com
  - Contains many channels, e.g. Biocontainers (http://biocontainers.pro/)
- There are a few other registries
- Sylabs (Singularity) also has a hub (library)
  - Not that much used



How to find a container

- Google or hub.docker.com search
  – E.g. “blast docker”
- Use singularity (Sylabs library) search

```
$ singularity search lammps
Found 4 containers for 'lammps'
        library://lammps/default/la
mmps_development
                Tags: centos7
centos8 fedora30_mingw
fedora32_mingw ubuntu16.04
ubuntu18.04 ubuntu18.04_amd_rocm
ubuntu18.04_amd_rocm_cuda
ubuntu18.04_intel_opencl
ubuntu18.04_nvidia ubuntu20.04
```



Run vs. pull vs. build

- pull will download the container and create sif file
- build does the same but names sif file and has more options
- run/exec will download if needed and run

```
$ apptainer pull docker://ubuntu:latest
```

- Singularity pulls the Docker layers to ~/.singularity, but puts sif file to local directory

```
$ apptainer build my_ubuntu.sif docker://ubuntu:latest
$ ls
my_ubuntu.sif   ubuntu_latest.sif
$ apptainer exec ubuntu_latest.sif /bin/bash
$ apptainer shell ubuntu_latest.sif
```

With Singularity use the `singularity` command.

Files in and out of the container

- Let's create a Python script

```
echo 'print("hello world from the outside")' > myscript.py
```

- Now run this script using the system's Python

```
python ./myscript.py
```

- Now run the script in the DockerHub python container

```
apptainer exec docker://python python ./myscript.py
```

…Conclusion: Scripts and data can be kept inside or outside the container. In some instances (e.g., large datasets or scripts that will change frequently) it is easier to containerize the software and keep everything else outside.

Some useful tips

- Binding mount points

```
$ export APPTAINER_BINDPATH="/tmp"
$ apptainer shell -B /scratch/local/$USER:/tmp ubuntu_python.img
```

- Specifying shell

```
$ export APPTAINER_SHELL=/bin/bash
$ apptainer shell -s /bin/bash ubuntu_python.img
```

- More specialized topics – ask us
  - Using environment modules from the host
  - Using GPUs, MPI over InfiniBand

Using GPUs

- Need to bring in the Nvidia driver stack
  - --nv runtime flag brings the drivers from the host
    - Still need to have a compatible CUDA installed in the container (older than or the same as the driver)
- On a GPU node, can e.g. execute:

```
apptainer exec --nv docker://tensorflow/tensorflow:latest-gpu python -c
"import tensorflow as tf; tf.config.list_physical_devices()"
```

Using MPI and InfiniBand

- Need to bring the IB stack in the container
  – Some people bring the needed IB libraries from the host
  – For Ubuntu we prefer to install the Ubuntu stack
  – https://github.com/CHPC-UofU/Singularity-ubuntu-mpi
- MPI
  – Build inside the container with IB, or use CHPC's modules
  – Prefer MPICH and derivatives, OpenMPI is very picky with versions
  – If using OS stock MPI, then make sure to LD_PRELOAD or LD_LIBRARY_PATH ABI compatible libmpi.so with InfiniBand
  – https://github.com/CHPC-UofU/Singularity-meep-mpi

Using Lmod from containers

- Many Linux programs are binary compatible between distros
  - Most installed binaries are (Intel, NVHPC tools, DDT, …)
- No need to install these in the container – use our NFS mounted software stack through Lmod
  - Need to have separate Lmod installation for Ubuntu due to some files having different location
- In the container
  - Install Lmod dependencies
  - Modify /etc/bash.bashrc to source our Lmod

https://github.com/CHPC-UofU/Singularity-ubuntu-python/blob/master/Singularity

Useful container repositories

- General HPC
  - Nvidia Containers - https://catalog.ngc.nvidia.com/containers
  - E4S – Extreme-scale Scientific Software Stack – https://e4s.io
    - 50 programs, incl. GPU, multiple Linux Distros
  - Many other projects
- Interpreted languages
  - R - Rocker - https://www.rocker-project.org/
  - Python – official DockerHub - https://hub.docker.com/_/python

Hands on – container commands in a module

- Follow our documentation:
  - https://www.chpc.utah.edu/documentation/software/singularity.php#exd
- Pull container
  - NGC's LAMMPS: https://catalog.ngc.nvidia.com/orgs/hpc/containers/lammps

```
$ mkdir ~/containers; cd containers; ml apptainer
$ apptainer pull lammps.sif docker://nvcr.io/hpc/lammps:29Sep2021
```

- Explore the container to find the program files

```
$ apptainer shell lammps.sif
$ which lmp
```

Hands on – container commands in a module

- Get a module file:

```
$ mkdir $HOME/MyModules/lammps
$ cd $HOME/MyModules/lammps
$ cp /uufs/chpc.utah.edu/sys/modulefiles/templates/container-template.lua 29Sep2021.lua
```

Modify the module file

```
-- path to the container sif file
local CONTAINER="/uufs/chpc.utah.edu/common/home/u0101881/containers/lammps.sif"
-- text array of commands to alias from the container
local COMMANDS = {"/usr/local/lammps/sm70/bin/lmp","/usr/local/lammps/sm70/bin/hpcbind"}
-- set to true if the container requires GPU(s)
local GPU = true
```

Hands on – container commands in a module

- Use module file:

```
$ module use $HOME/MyModules
$ module load lammps/29Sep2021
$ which lmp
$ mkdir -p $HOME/lammps/data; cd $HOME/lammps/data
$ wget https://lammps.org/inputs/in.lj.txt
$ lmp -in in.lj.txt

(to run on GPU)
$ lmp -k on g 1 -sf kk -pk kokkos cuda/aware on neigh full comm device
binsize 2.8 -var x 8 -var y 8 -var z 8 -in in.lj.txt
```

Building Singularity containers

Recall: container execution

- On **any system** with Apptainer/Singularity, even without administrative privilege, you can retrieve and use containers:
- Download a container from Docker Hub

```
apptainer pull docker://some_image
apptainer build mycont.sif docker://some_image
```

- Run a container

```
apptainer run mycont.sif
```

- Execute a specific program within a container

```
apptainer exec mycont.sif python myscript.py
```

- “Shell” into a container to use or look around

```
apptainer shell mycont.sif
```

- Inspect an image

```
apptainer inspect --runscript mycont.sif
```

When to build own containers

- Complex software dependencies
  - Especially Python and R packages
    - bioBakery – intricate dependencies of Python and R which did not build on CentOS
    - SEQLinkage – instructions to build on Ubuntu using its packages
- Quick deployment
  - Some Linux distros provide program packages while others don’t
    - paraview-python on Ubuntu via apt-get
- Deploying your own code or pipeline
- Modify or add onto an existing container

Container build strategy

- Start with a the basic container (e.g. ubuntu:latest from Docker)
- Shell into the container
  - Install additional needed programs
    - If they have dependencies, install the dependencies – google for the OS provided packages first and install with apt-get/yum if possible
  - Put the commands in the `%post` scriptlet
- Build the container again
  - Now with the additional commands in the `%post`
  - If something fails, fix it, build container again
- Iterate until all needed programs are installed

Two ways of building containers

- Build a container on a system on which you have administrative privilege (e.g., your laptop, singularity.chpc.utah.edu).
  - Pros: You can interactively develop the container.
  - Cons: Requires many GB of disk space, requires administrative privilege, must keep software up-to-date, container transfer speeds can be slow depending on personal network connection.
- Build a container on Sylabs Cloud
  - Pros: Essentially zero disk space required on your system, doesn't require administrative privilege, no software upgrades needed, easy to retrieve from anywhere, typically faster transfers from Sylabs Cloud to desired endpoint, interactive container development works.
  - Cons: Need to set up access to Sylabs Cloud, slower interactivity in the container development.

Two ways of building containers

- ~~Build a container on a system on which you have administrative privilege (e.g., your laptop, singularity.chpc.utah.edu).~~
  - ~~Pros: You can interactively develop the container.~~
  - ~~Cons: Requires many GB of disk space, requires administrative privilege, must keep software up-to-date, container transfer speeds can be slow depending on~~

Latest versions of Apptainer allow rootless container build

~~anywhere, typically faster transfers from Sylabs Cloud to desired endpoint, interactive container development works.~~

  - ~~Cons: Need to set up access to Sylabs Cloud, slower interactivity in the container development.~~

Container build process

- Create a writeable container

```
$ apptainer build --sandbox mycont ubuntu22.def
```

  - This creates a container directory called `mycont`

- If additional installation is needed after the build
  - Shell into the container and do the install manually

```
$ apptainer shell -w -s /bin/bash mycont
```

  - Execute what's needed, modify container definition file, repeat

- When done, create a production container

```
$ apptainer build ubuntu22.sif ubuntu22.def
```

Container definition file (a.k.a. recipe)

- Defines how the container is bootstrapped
  - Header – defines the core OS to bootstrap
  - Sections – scriptlets that perform additional tasks
- Header
  - Docker based (faster installation)

```
BootStrap: docker
From: ubuntu:latest
```

  - Linux distro based

```
BootStrap: debootstrap
OSVersion: xenial
MirrorURL: http://us.archive.ubuntu.com/ubuntu/
```

```
Bootstrap:docker
From:ubuntu:latest

%labels
MAINTAINER Andy M

%environment
HELLO_BASE=/code
export HELLO_BASE

%runscript
echo "This is run when you run the image!"
exec /bin/bash /code/hello.sh "$@"

%post
echo "This section is performed after you bootstrap to build the image."
mkdir -p /code
apt-get install -y vim
echo "echo Hello World" >> /code/hello.sh
chmod u+x /code/hello.sh
```

Definition file sections

- `%setup` Runs on the host
  - Install host based files (e.g. GPU drivers)
- `%post` Runs in the container
  - Install additional packages, configure, etc
- `%runscript` Defines what happens when container is run
  - Execution commands
- `%test` Runs tests after the container is built
  - Basic testing

Definition file sections cont'd

- `%environment` Definition of environment variables
- `%files` Files to copy into the container
- `%labels` Container metadata
- `%help` What displays during `apptainer help` command

- More details at https://apptainer.org/docs/user/main/definition_files.html

Building a container CHPC interactive node

1. Log in to Frisco: `ssh uxxxxxx@frisco1.chpc.utah.edu`
2. Create a recipe file for your container, name it "Singularity", e.g.
   ```
   $ nano Singularity
   Bootstrap: docker
   From: alpine:3.9
   %post
   apk update; apk upgrade; apk add bash
   ```
   To exit and save type [ctrl-x], then "y", then [enter].
3. Initialize Apptainer and build container
   ```
   $ ml apptainer
   $ apptainer build alpine.sif Singularity
   ```
4. Verify that the container is available by opening shell in it
   ```
   $ apptainer shell alpine.sif
   ```

Troubleshooting and Caveats

Host/container environment conflicts

- Container problems are often linked with how the container "sees" the host system. Common issues:
  - The container doesn't have a bind point to a directory you need to read from / write to
  - The container will "see" python libraries installed in your home directory (and the same is true for R and other packages). If this happens, set the PYTHONPATH environment variable in your job script so that it points to the container paths first.

    `export PYTHONPATH=<path-to-container-libs>:$PYTHONPATH`

    - or use the `--cleanenv` option

- To diagnose the issues noted above, as well as others, "shelling in" to the container is a great way to see what's going on inside.
- Also, look in the singularity.conf file for system settings (can't modify).

Pull and build errors

- Sometimes build fails due to corrupted locally cached image layer files. Use `apptainer cache list` followed by `apptainer cache clean` to clean up the old layers.

- When building ubuntu containers, failures during *%post* stage of container builds from a recipe file can often be remedied by starting the *%post* section with the command "apt-get update". As a best practice, make sure you insert this line at the beginning of the *%post* section in all recipe files for ubuntu containers.

Overlays

- Overlays are additional images that are ”laid” on top of existing images, enabling the user to modify a container environment without modifying the actual container. Useful because:
  - Overlay images enable users to modify a container environment even if they don’t have root access (though changes disappear after session)
  - Root users can permanently modify overlay images without modifying the underlying image.
  - Overlays are a likely way to customize images for different HPC environments without changing the underlying images.
  - More on overlays: https://www.sylabs.io/guides/3.6/user-guide/persistent_overlays.html

Moving containers

- You've built your container on your laptop. It is 3 Gigabytes. Now you want to move it to CHPC to take advantage of the HPC resources. What's the best way?
- Containers are files, so you can transfer them to CHPC just as you would a file:
  - Command line utilities (scp, sftp)
  - Globus or rclone (recommended)
    https://www.chpc.utah.edu/documentation/software/rclone.php
    https://www.chpc.utah.edu/documentation/software/globus.php
  - For more on data transfers to/from CHPC:
    https://www.chpc.utah.edu/documentation/data_services.php

Resources

- http://sylabs.io
- http://cloud.sylabs.io
- https://apptainer.org/
- https://hpc.github.io/charliecloud/
- https://www.chpc.utah.edu/documentation/software/containers.php
- https://github.com/CHPC-UofU

Questions?