Installing containerized software on Alpine

Research Computing
UNIVERSITY OF COLORADO BOULDER

Installing software on Alpine with Conda and Mamba

Date: February 27, 2024

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- Website: www.rc.colorado.edu
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu
- Survey: http://tinyurl.com/curc-survey18

Slides

https://github.com/ResearchComputing/containerized_software_alpine_primer

Learning Objectives

- What is a software container?
- How can I find existing software containers?
- How can I use a container on Alpine?
- How can I build a container on Alpine?

Session Overview

Introduction
- Installing software on CURC systems
- Defining containers
- Description of Apptainer

Setting up Conda on Alpine
- Logging in
- Using conda for the first time: creating the ~/.condarc file
- Starting an interactive session and activating conda

Creating and Modifying Virtual Environments with Conda
- Creating/activating/modifying a python environment
- Useful conda commands and paths

Using Conda Virtual Environments
- In HPC jobs
- In OnDemand Jupyter

Strategies for installing complex Virtual Environments (Discussion only)
- Channels
- Resolving conflicts upon environment creation
- Mamba

Building Software on Alpine

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

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

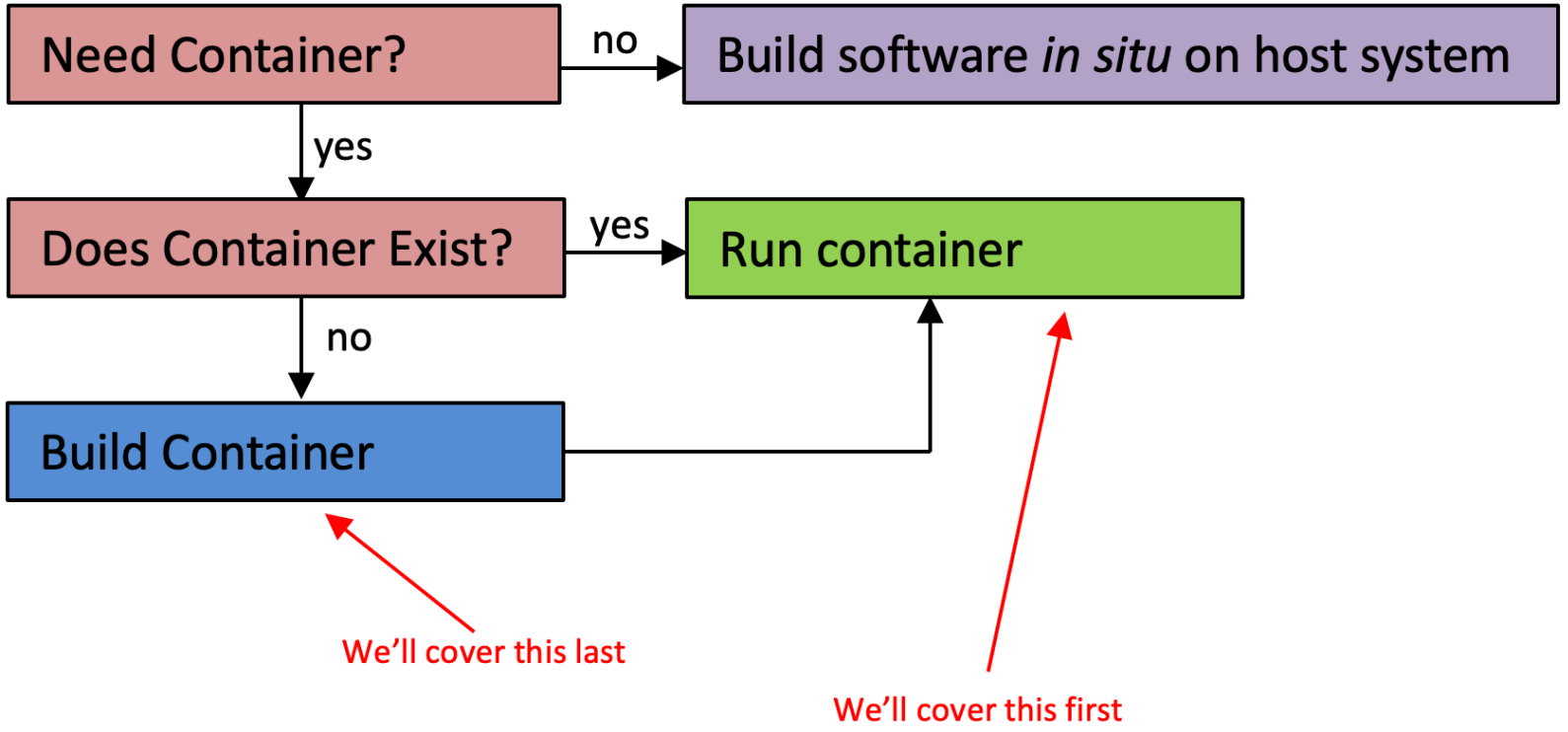
What is a Container?

- A container is a portable environment that packages some or all of the following: an operating system, software, libraries, compilers, data, and workflows. Containers enable:
  - Mobility of compute
  - Reproducibility (software and data)
  - User Freedom

Containerization Software

- Docker 
  - Well-established
  - Most widely used
  - Millions of containers already available on DockerHub
- **Apptainer** 
  - Formerly "Singularity"
  - HPC-safe
- Others

Making the decision to containerize



Logging into CU Research Computing

login to CURC via your terminal:

```
ssh monaghaa@login.rc.colorado.edu
```

…or login to CURC via your browser:

https://ondemand-rmacc.rc.colorado.edu

(once logged in, navigate to **Clusters -> Alpine shell**)

Additional information:
https://curc.readthedocs.io/en/latest/access/logging-in.html
https://curc.readthedocs.io/en/latest/gateways/OnDemand.html

Start a compute session

Start a session on an Alpine compute node with **acompile**:

```
[monaghaa@login11 ~]$ acompile --help
[monaghaa@login11 ~]$ acompile --ntasks=4 --time=90:00
…
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer --help
```

Note: when you login to CURC you'll be on a ***login*** node. You'll need to be on a ***compute*** node to use apptainer. The **acompile** command allows you to quickly start an interactive job on a compute node.

Additional information:
https://curc.readthedocs.io/en/latest/clusters/alpine/alpine-hardware.html#partitions

Let's run our first container!

Invoke "R" statistical software in a pre-existing container:

```
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer exec $CURC_CONTAINER_DIR/debian_r_4_2_2.sif R
> 1+2
> quit ()

[monaghaa@c3cpu-a5-u28-1 ~]$ ls $CURC_CONTAINER_DIR/    # ← what the heck is in this directory?
```

Let's run an external R script with the container

```
[monaghaa@c3cpu-a5-u28-1 ~]$ cd /scratch/alpine/$USER
[monaghaa@c3cpu-a5-u28-1 ~]$ git clone https://github.com/ResearchComputing/containerized_software_alpine_primer
[monaghaa@c3cpu-a5-u28-1 ~]$ cd containerized_software_alpine_primer/examples
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer exec $CURC_CONTAINER_DIR/debian_r_4_2_2.sif Rscript prime_functions.R
```

Key Apptainer Commands

exec: Execute a command to your container

run: Run your image as an executable (behavior must be predefined)

build: Build a container on your user endpoint or build environment

pull: pull an image from Docker or Singularity Hub

inspect: See labels, run and test scripts, and environment variables

shell: Shell into your image

Now let's explore a container

Shell into the container:

```
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer shell $CURC_CONTAINER_DIR/gmtsar_v6.2.sif
Apptainer> cat /etc/os-release   # what operating system is in the container?
Apptainer> ls /usr/local # what do you see?
Apptainer> exit
```

Inspect how the container was built:

```
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer inspect -d $CURC_CONTAINER_DIR/gmtsar_v6.2.sif
```

…now let's look more closely at a container definition file

Container definition file

lolcow.def

```
Bootstrap: docker
From: ubuntu:20.04

%post
    apt-get -y update
    apt-get -y install cowsay lolcat

%environment
    export LC_ALL=C
    export PATH=/usr/games:$PATH

%runscript
    date | cowsay | lolcat
```

Example source: https://apptainer.org/docs/user/latest/definition_files.html

Now let's build and run a container

```
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer build lolcow.sif lolcow.def
…will take a couple of minutes

# run default container behavior
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer run lolcow.sif

# run your own script from container
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer exec lolcow.sif /bin/sh lolcow.sh
```

Now let's pull and run a Docker container

```
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer pull cp2k.sif docker://cp2k/cp2k:latest
…will take a couple of minutes

# run at command line:
[monaghaa@c3cpu-a5-u28-1 ~]$ apptainer run cp2k.sif cp2k -o md300.out md300.inp

# schedule a job
[monaghaa@c3cpu-a5-u28-1 ~]$ sbatch run_cp2k.sh
```

More complex topics (if time allows)

- Bind mounting external directories
- Using containers on GPUs
- Using containers with MPI

Thank you!

Survey and feedback

http://tinyurl.com/curc-survey18