Managing Research Workflows with Singularity Containers: Part 1

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Slides available for download at
https://github.com/rctraining/Singularity_Short_Course_Spring_2018

Adapted from a presentation by Martin Cuma (U. Utah; 1) and materials from https://singularity.lbl.gov/ and https://www.singularity-hub.org

Outline

- Introduction to Containers
- Singularity Commands and options
- Hands-on Examples
- Summary

Introduction to Containers

What is a container?

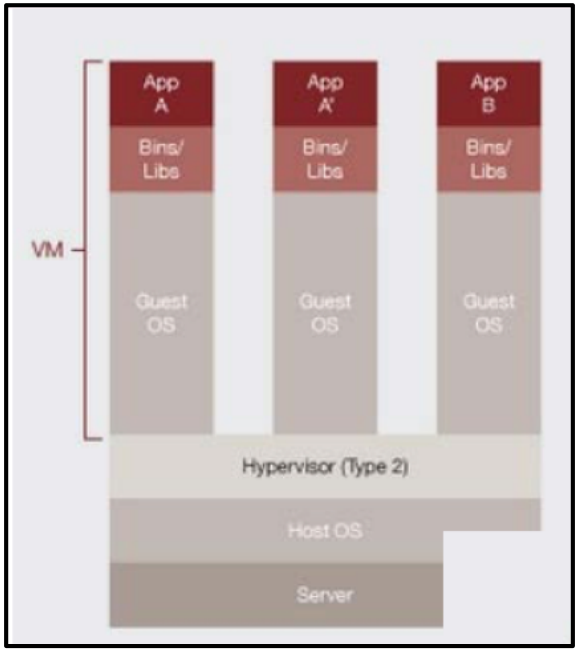
A container is a portable environment that packages some or all of the following: an operating system, software, libraries, compilers, data and workflows. Containers enable:

- Mobility of Compute
- Reproducibility (software and data)
- User Freedom

Virtualization (1)

Hardware virtualization (not used by containers!)

- Can run many OS's on same hardware (machine)
- E.g., VirtualBox, VMWare

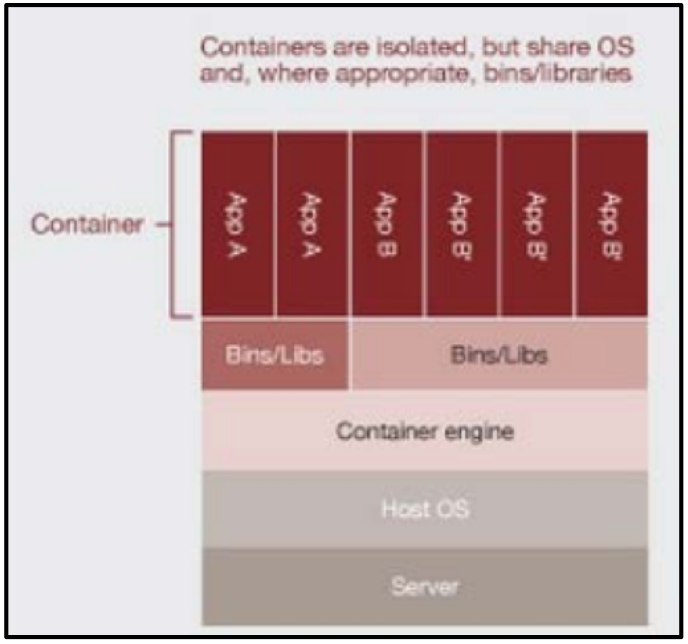


Material courtesy: M. Cuma, U. Utah

Virtualization (2)

OS-level virtualization (used by containers!)

- Can run many isolated OS instances (guests) under a server OS (host)
- Also called containers
- E.g., Docker, Singularity



Best of both worlds: isolated environment that user wants, but can leverage host OS resources (network, I/O partitions, etc.)

Material courtesy: M. Cuma, U. Utah

Why Singularity?

- Singularity is a comparably safe container solution for HPC
  - User is same inside/outside container
  - User has cannot escalate permissions without administrative privilege
- Can support MPI and GPU resources on HPC (scaling)
- Can use HPC filesystems
- Supports the use of Docker containers
- Container is seen as a file, and can be operated on as a file

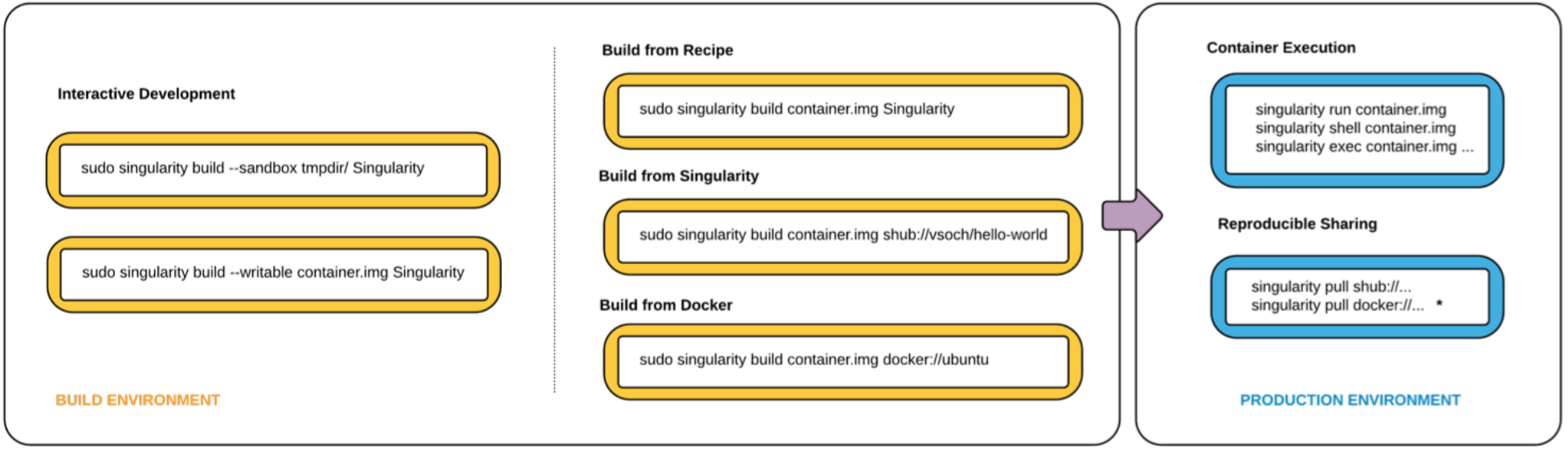
Singularity commands and options

Interactive development

Building

Running

The Singularity workflow



* Docker construction from layers not guaranteed to replicate between pulls

https://singularity.lbl.gov

Interactive development

Within your build environment (a laptop, workstation, or a server that you control): develop and test containers

- using --sandbox (build into a writable *directory*)
    - `sudo singularity build --sandbox tmpdir/ mycont.def`

- or using --writable (build into a writable *ext3* image)
    - `sudo singularity build --writable tmp.img mycont.def`

Building containers

After development, within your build environment (a laptop, workstation, or a server that you control): build your production containers with a *squashfs* filesystem...

- Build from a "recipe" that you developed.
  - `sudo singularity build mycont.img mycont.def`
- Build from an existing container on Singularity Hub
  - `sudo singularity build mycont.img shub://somewhere`
- Build from an existing container on Docker Hub
  - `sudo singularity build mycont.img docker://somewhere`

Container Formats

- **squashfs**: the default container format is a compressed read-only file system that is widely used for things like live CDs/USBs and cell phone OS's
- **ext3**: (also called `writable`) a writable image file containing an ext3 file system that was the default container format prior to Singularity version 2.4
- **directory**: (also called `sandbox`) standard Unix directory containing a root container image
- **tar.gz**: zlib compressed tar archive
- **tar.bz2**: bzip2 compressed tar archive
- **tar**: uncompressed tar archive

https://singularity.lbl.gov

Running containers

Now, on ***any system*** with Singularity, even without administrative privilege, you can retrieve and use containers:

- Download a container from Singularity Hub or Docker Hub
  - `singularity pull shub://some_image`
  - `singularity pull docker://some_image`
- Run a container
  - `singularity run mycont.img`
- Execute a specific program within a container
  - `singularity exec mycont.img python myscript.py`
- "Shell" into a container to use or look around
  - `singularity shell mycont.img`
- Inspect an image
  - `singularity inspect --runscript mycont.img`

Singularity Commands

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

exec: Execute a command to your container

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

pull: pull an image from Docker or Singularity Hub

run: Run your image as an executable

shell: Shell into your image

https://singularity.lbl.gov

Hands-on Examples

Building a container from Singularity Hub

Building a container from a recipe

Building a container from Docker Hub

Building a container *on* Singularity Hub

Caveats

For the sake of expediency, we will build containers based on Ubuntu Linux. Most other variants/versions of Linux are available.

We will do everything on our 'root' system in this session; i.e., our laptop or desktop computer. In Part 2 (next week) we will run on RMACC Summit, a system on which we do not have root access.

We don't cover a number of topics. E.g.,

- "instances" (running services from containers in the background)
- Other containerization software that can work on HPC
    - Shifter, Charliecloud (neither presently installed on Summit)

https://singularity.lbl.gov

Start your Linux VM so that you can run Singularity

Once you've installed Singularity on your machine (assuming Mac or Windows):

```
$ mkdir singularity-vm
$ cd singularity-vm
$ vagrant init singularityware/singularity-2.4
$ vagrant up
$ vagrant ssh
```

If you are on Linux, you don't need to start a VM

Ex1: Build a container from Singularity Hub

…let's build a container from existing image

```
$ sudo singularity build --writable hello.img
shub://vsoch/hello-world
```

…let's run the default program in the image

```
$ singularity run hello.img
```

…let's look at the recipe

```
$ singularity inspect -d hello.img
```

…now let's shell in and modify the image

```
$ singularity exec hello.img /bin/bash /rawr.sh
```

…now let's modify the image

```
$ sudo singularity shell --writable hello.img
```

… now let's run our new program

```
$ singularity exec hello.img /bin/bash hello.sh
```

Ex2: Building a container from a recipe (1)

Header

Metadata

Runtime environment variables

Default program at runtime

Where software and directories are installed at buildtime

```
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
```

Ex2: Building a container from a recipe (2)

See http://singularity.lbl.gov/docs-recipes for more.

Now let's build and run a container from our recipe.

```
$ git clone
https://www.github.com/monaghaa/singularity_git_tutorial

$ cd singularity_git_tutorial

$ sudo singularity build --writable mycont.img Singularity

$ singularity run mycont.img
```

Ex3: Build a container from Docker Hub

…let's build a container from existing image

```
$ sudo singularity build --writable python.img
docker://python:latest
```

…let's run the default program in the image

```
$ singularity exec python.img python
```

…let's add the numpy package to the container

```
$ sudo singularity shell -w python.img
```

Ex4: Build a container on Singularity Hub (basic steps)

1. Create a github repository for your container or class of containers.
2. Create a recipe file for whatever you want your container to be
3. Name it “Singularity”
4. Upload it to your github repository
5. Log into Singularity Hub using your github username/password
6. Choose “Add Collection”
7. Select the github repository
8. The container will build automatically.
9. Additional details at: *https://github.com/singularityhub/singularityhub.github.io/wiki*

Common Issues

Failures during container builds that are attributed (in the error messages) to *tar.gz files are often due to corrupt tar.gz files that are downloaded while the image is being built from layers. Removing the offending tar.gz file will often solve the problem.

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.

https://singularity.lbl.gov

Thank you!

Please fill out the survey:
http://tinyurl.com/curc-survey16

My contact information:
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Additional learning resources:
Slides and Examples from this course:
https://github.com/rctraining/Singularity_Short_Course_Spring_2018

Web resources:
https://singularity.lbl.gov/user-guide *(user guide for Singularity)*
https://www.singularity-hub.org/ *(Singularity Hub)*