# Containerization for R&D Applications (Part 1!)

Daniel Trahan

*Daniel.Trahan@colorado.edu*

Please sign in:
https://tinyurl.com/y4aks9zs

Slides and exercises available for download at:
***https://github.com/ResearchComputing/CONTAINER_TUTORIAL_FALL_2020***

# Outline

## Part 1: Container fundamentals and Docker (11/12/20)

- Introduction to containers
- Docker commands and options
- Hands-on: Running Docker containers on your personal Machine
- Hands-on: Building Docker images
- Hands-on: Practical Application

## Part 2: Containers for HPC with Singularity (11/19/20)

- Singularity commands and options
- Hands-on: Running containers
- Building containers
- Special cases: Running containers for MPI and GPU jobs

# Introduction to Containers

Seacontainersales.com

# What is a container?

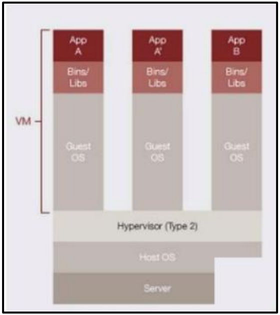
A container is a portable environment that packages some or all the following: an operating system, software, libraries, compilers, data and workflows. Containers enable:

- 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



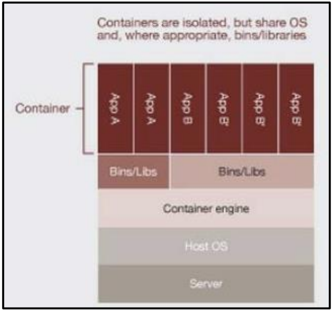
*Material courtesy: M. Cuma, U. Utah*

# 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*

# Containerization software

- Docker
    - Part 1 focus of today's tutorial
    - Well established – largest user base
    - Has Docker Hub for container sharing
    - Problematic with HPC
- Singularity
    - Part 2 focus of next week tutorial
    - Designed for HPC
- Charliecloud; Shifter
    - Designed for HPC
    - Based on Docker
    - Less user-friendly

# Installing Docker

- Docker Community Edition
  - Windows: Windows 10 Professional or Enterprise
  - Mac: OS X El Capitan 10.11 or later
  - Linux
- Docker toolbox
  - Legacy solution for Windows and Mac for versions that do not meet the version requirements.
  - Utilizes the Virtual Box hypervisor for virtualization
  - For this tutorial, Windows users regardless of version will use Docker toolbox

# Why Docker?

- Probably the most popular containerization software
- Offers a variety of prebuilt images including:
  - Python
  - Perl
  - NodeJS
  - Ubuntu
- Very well documented with a large community creating and supporting docker images.
- DockerHub

# Docker Nuts and Bolts

- Docker runs on a concept of images and containers.
  - ***Images***: Saved snapshots of a container environment.
    - Made from Dockerfile or pulled from Docker Hub
    - Stored in the Docker cache on your disk
  - ***Containers***: Instances of images that are generated by Docker when an image is 'run'
    - Instance of image running in memory
    - Ephemeral Instances that cannot be continued
    - Can be run interactively

# Docker Commands

- Docker Commands are usually in the form of:

```
docker <sub-command> <flags> <target/command>
```

- Examples:

```
docker run -it myimage
docker container ls
docker image prune
```

# Running Docker Containers

- Run a docker image as a container:

```
docker run <image-name>
```

- Run a docker image interactively:

```
docker run -it <image-name>
```

- If an image is not on the system, then Docker will search Dockerhub to see if the image exists.
- Specify commands after your image to execute specific software in your container.

```
docker run <image-name> <program>
```

# Containerized Hello World

- Let's start with something simple:
  - Docker "Hello, World!"
    - Relatively small image
    - No dependencies
    - Built as a general test case
- Command:

```
docker run hello-world
```

# Docker Image and Container Commands

| Image Commands | |
|---|---|
| `docker image ls` | List docker images stored in cache: |
| `docker image rm <image>`<br>`docker rmi <image>` | Remove (an) image(s): |
| `docker image prune` | Remove unused images |

| Container Commands | |
|---|---|
| `docker container ls` | List docker containers currently running: |
| `docker container rm <container>`<br>`docker rm <container>` | Remove (an) container(s): |
| `docker container prune` | Remove all stopped containers |

# Docker Utility Commands

| Commands | |
|---|---|
| `docker info` | Shows Docker system-wide information |
| `docker inspect <docker-object>` | Shows low-level information about an object |
| `docker config <sub-command>` | Manage docker configurations |
| `docker stats <container>` | Shows container resource usage |
| `docker top <container>` | Shows running processes of a container |
| `docker version` | Shows docker version information |

- More details and commands can be found *on the docker documentation page*

# Demo 1: Running Containerized Python

# Demo 1: Python

- Running the Python docker container will pull Python from Docker Hub:

```
docker run python:3.7.2-slim
```

- ...did it work?
- Run your python image interactively:

```
docker run –it python:3.7.2-slim
```

- This puts us into a python interpreter, where you can run python code containerized in its own environment.

# Building Docker Containers

- To build a docker container, we need a set of instructions Docker can use to set up the environment.
  - Dockerfile
- Once we set up our dockerfile we can use the command

```
docker build –t <image-name> .
```

- Then we can run the image with our `docker run` command

```
docker run <image-name>
```

# Demo 2: Building an Ubuntu Container

# Demo 2: Setup

Dockerfiles and test files are provided for this workshop. We can pull the files from a github repository as such:

1. Navigate to your home directory

   ```
   cd ~
   ```

2. Clone the repository

   ```
   git clone
   https://github.com/ResearchComputing/Container_tutorial_Spring_2020
   ```

# Demo 2: Ubuntu w/ GCC

- For this first example we will be building a custom Ubuntu image that will provide a location to run the GNU Compiler Collection.
- Dockerfile provided
- Need to build:
  1. Navigate to the directory:
     ```
     cd ~/Container_tutorial_Spring_2020/dockerdemo/ubuntu-gcc
     ```
  2. Build the docker image with:
     ```
     docker build –t happy-gcc .
     ```
  3. Run the docker image as a container:
     ```
     docker run –it happy-gcc
     ```

# Editing Docker Images

- Suppose you have an existing docker image and want to make changes…
  - Rebuild Dockerfile!
    - Usually a bit cumbersome
    - No Dockerfile?
- Use docker commit!

```
docker run -it <image-name> bash #or any shell...
```

- Then commit it to the image

```
docker commit <image-id> <image>
```

# Mounting and Accessing files

- So now that we have a working container, how can we access the test files we downloaded?
    - Mounting directories: Bind Mount
        - Allows the docker container to access files on the host OS
        - Choose host's **source directory**, files in the directory will be moved to the container's **target directory**
            - ***Source Directory***: Directory on the host system. Never within a container.
            - ***Target Directory***: Directory in the Docker Container. Never on the host system.
        - A flag set within the `docker run` command:

```
docker run --mount type=bind,source=<source>,target=<target> <image>
```

# Mounting and Accessing files

- Mounting directories: Volume Mount
  - Same concept, but volumes are stored within docker cache.
  - Create Docker volumes in your terminal and link your volume directory
  - Similarly linked through the `docker run` command.

```
docker run --mount type=volume,source=<volume>,target=<target> <image>
```

# Demo 2 (Cont.): Mounting

- Returning to our demo, can we give our container access to our test files?
- Let's use a bind mount!
- In the directory where our Dockerfile lives... use this command (all on one line):

```
docker run –it --mount
type=bind,source=$(pwd)/source,target=/target happy-gcc
```

- We can `cd /target` and run our test files!
- Command:

```
gcc hello.c -o hello.exe
./hello.exe
```

# Demo 3: NCL container

- For this next example we will building a Docker image that will run the NCAR Command Language (NCL).
- Dockerfile provided
- Same process as before:
  1. Navigate to the Dockerfile found at:
     ~/Container_tutorial_Spring_2020/dockerdemo/ncl
  2. Build your docker file as an image titled "bright-ncl"
  3. Run your docker image as a container
- Can we test a sample script?

# Dockerhub

- The place where containers live!
- Dockerhub is a Docker hosted library of public and private Docker images.
    - Free and unlimited public images
    - 1 free private repository
- Great for hosting images for fellow researchers
- Commands similar to git

# Dockerhub Commands

- Download and upload docker images with ease.
  - docker run <image>
  - docker pull <image>
- Uploading a little more complicated...
  - Sign in with:

    docker login
  - List docker images with:

    docker image ls
  - Tag your image:

    docker tag <image-id> <your-username>/<image-name>:<tag>
  - Push!

    docker push <your-username>/<image-name>

# Docker-Compose

- Utility that can create and install docker images.
- Builds docker images based on a docker-compose.yml file.
    - YAML: *YAML Ain't Markup Language*
    - Data serialization language
    - Describes containers you wish to build with what features.
- Not a docker command!

# Docker-Compose Commands

- Build all containers in YAML file:

  docker-compose build

- Build and run all containers in YAML file:

  docker-compose up

- List all containers in YAML file:

  docker-compose images

- Run a one-off command from a container:

  docker-compose run <container-name> <command>

# Thank you!

Please fill out the survey:
*http://tinyurl.com/curc-survey18*

Contact information:
*Daniel.Trahan@Colorado.edu*

Additional learning resources:

*Slides and Examples from this course:*
*https://github.com/ResearchComputing/CONTAINER_TUTORIAL_FALL_2020*

*Web resources:*
*https://training.play-with-docker.com* *(docker online training materials)*
*https://hub.docker.com* *(Docker Hub)*