Enabling Reproducibility with Docker

Research Computing
UNIVERSITY OF COLORADO **BOULDER**

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Enabling Reproducibility with Docker

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- *RC Homepage: https://www.colorado.edu/rc/*
- *RC Docs: https://curc.readthedocs.io/en/latest/*
- *RC Helpdesk: rc-help@colorado.edu*

- Course Materials: https://github.com/ResearchComputing/Containers_Spring_2022

Outline

- Part 1: Container fundamentals and Docker (4/7/2022)
  - Reproducibility and the Case for Containers
  - Containers
  - Docker
    - Images and Containers
    - Commands
    - File Access
    - Building Docker Images
    - DockerHub
- Part 2: Containers for HPC w/ Singularity (4/14/2022)

Tutorial Files:

- This tutorial will have interactive components
- If you would like to participate in the demos provided for this tutorial then first clone the test files from GitHub to your desired location:

1. Navigate to a desired directory
2. Clone the repository:

```
git clone https://github.com/ResearchComputing/Containers_Spring_2022.git
```

3. Navigate into the directory and store the path into a variable:

```
cd Containers_Spring_2022
export CONTAINER_ROOT=$(pwd)
```

Reproducibility and Research

- Scientific Software is often challenging to work with
  - Difficult installation
  - Low support from the developers
  - Very outdated
  - Complex Dependency trees
- Because of this it's often desired for a software to be repeatable and accurate.
- *But installs are only done once. Why should I care about reproducible applications.*

Reproducibility and Research

- Research is Collaborative
  - Team members work together to get projects done.
  - Reproducibility ensures all members of a team can provide productivity towards a project.
- Research is Correcting
  - Research is hard
  - Academic reviews are commonplace
  - Someone may wish to accurately reproduce your work
- Research is Continuous
  - You may be working on a single project for a long period of time
  - What happens in you move, but bring your work to another system?

Options for reproducibility

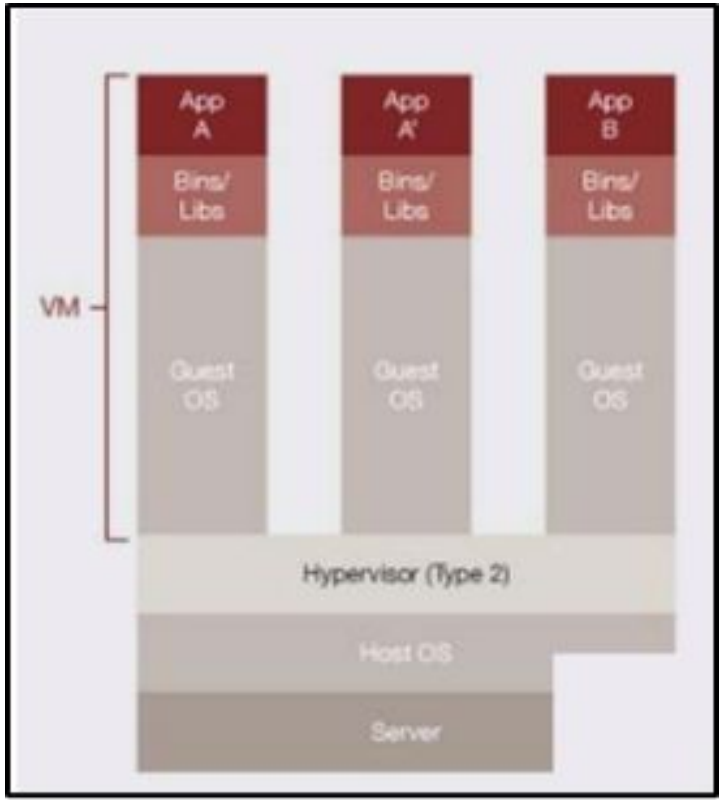
- Lots of options!
  - Detailed instructions
  - Software bundles
  - Virtual Environments
    - Python, Anaconda, Spack
- But do they really enable accurate reproducibility?
  - Incorrect installs?
  - Hardware or OS?
  - Performance?

Containers

- A Container is an isolated environment: packaged bundle of libraries, dependencies, and files that runs as a process under a host OS
- Containers use an application on the host operating system called a Container Manager
    - Manages operating system and libraries run as containers
    - Similar to virtual machines, but does not need dedicated CPUs memory or storage

Virtualization (1)

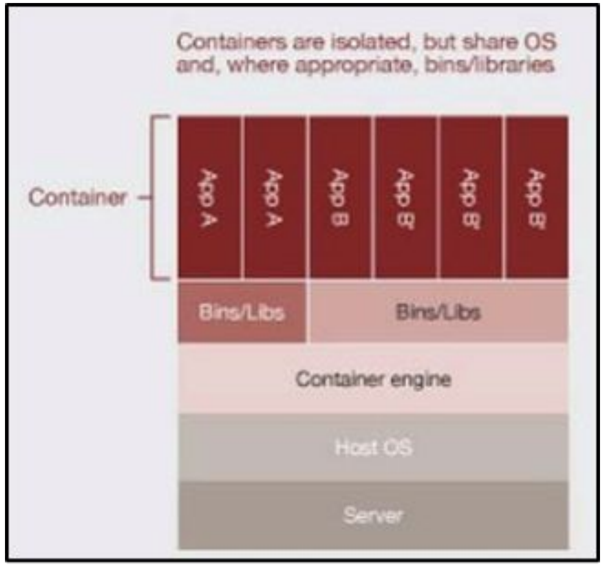
- Virtualization is a technology that utilizes software to abstract components of a technology
- Common application is Hardware Virtualization
  - Virtual Machines
    - Partitions off Memory, CPU, GPU, and Storage
    - Runs a virtual OS
    - Runs software on the virtualized machine
  - *Examples: VMware, Virtualbox*



Material courtesy: M. Cuma, U. Utah

Virtualization (2)

- Another use of virtualization is in OS Level Virtualization
  - Can run many isolated guest OS instances under a host OS kernel
  - This virtualization is what is used by Docker and other container software.
  - Virtualizing *software*, not *hardware*
  - Share a kernel
  - Best of both worlds!
    - Isolated environments
    - No hardware partitioning



Material courtesy: M. Cuma, U. Utah

Containerization Software

- Docker
  - Well established – largest user base
  - Has Docker Hub for container sharing
  - Problematic with HPC (Fix incoming!)
- Singularity
  - Designed for HPC
  - Second largest user base
  - Developed for scientific use
- Charliecloud; Shifter
  - Designed for HPC
  - Based on Docker
  - Less user-friendly

Installing Docker

- Docker Desktop
  - Comfy GUI to help keep track of containers and images!
  - Available on all operating systems (*beta on Linux*)
  - Windows users can enable WSL2 support following the instructions here: https://docs.docker.com/docker-for-windows/install/

- Docker hosted lab environment (Need Docker account, limited availability)
  - https://labs.play-with-docker.com/

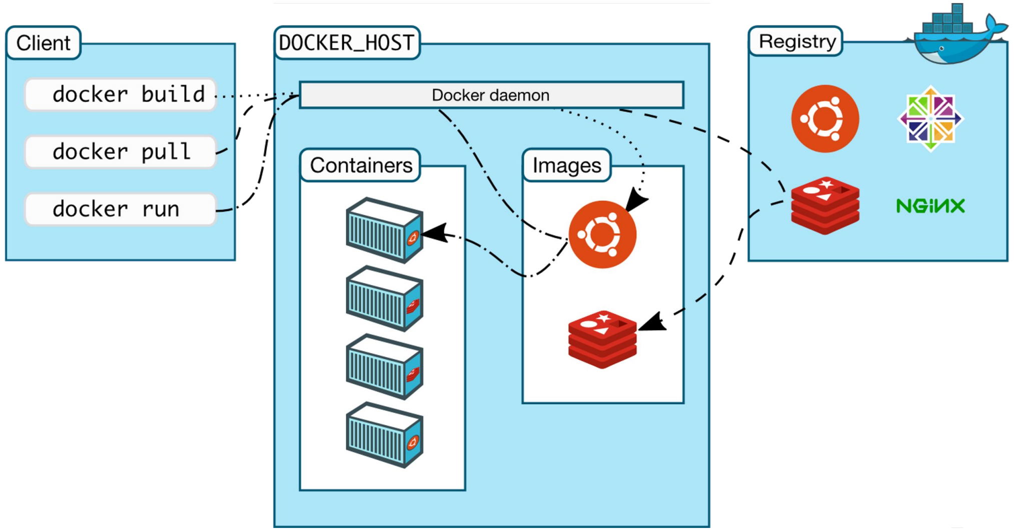
- Docker toolbox
  - Legacy solution for Windows and Mac for versions that do not meet the version requirements.
  - Utilizes the Virtual Box hypervisor for virtualization

Docker: 3 main components

- **Docker File**
  - Like DNA, code that tells docker how to build an image
- **Image**
  - Snapshot of your software along with all of its dependencies (down to OS level)
  - Immutable (mostly) and can be used to spin up multiple containers
- **Container**
  - Running instances of images that are isolated and have their own sets of environments and processes
  - Actual software running in the real world

Docker Nuts and Bolts

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



Docker ‘Hello World’

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

```
docker run hello-world
```

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
```

Launching a Docker Container

- Launch 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, and pull it down locally
- Specify commands after your image to execute specific software in your container.

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

Example:

```
docker run -it ubuntu bash
```

Listing Containers

- When a container is run it is assigned a name, an ID, name of the image used to run the container, current status.

- List all currently running containers

```
docker ps
```

- List all containers

```
docker ps -a
```

Stopping/Removing a container

- You can stop a container using the “stop” command:

  ```
  docker stop <name or ID>
  ```

  If you don’t know the docker name or id you can list containers

- If you don’t want a stopped container taking up space you can remove it with the remove command:

  ```
  docker rm <name or ID>
  docker container rm <name or ID>
  ```

Images

- To see a list of images (templates) for our container:

```
docker images
docker image ls
```

- To remove an image:

```
docker rmi <name>
docker image rm <name>
```

- To download an image but *not* run an image:

```
docker pull <name>
```

Exploring a Docker Container

- Docker containers are running tiny operating systems!
- We can explore the operating system by invoking a shell

```
docker run -it ubuntu bash
```

- This command launches the ubuntu Docker container with the command ‘bash’

- We can also run a command on an already running container with the “docker exec” command:

```
docker run -d ubuntu sleep 100
docker exec <container-id> cat /etc/*release*
```

Demo 1: Running a Container

Demo 1: GROMACS

- GROMACS is a molecular dynamics application that can often be a complex and challenging installation for the average user. Linux and Mac only
  - Dense Documentation
  - Software requires compilation
- Luckily, this can be trivialized with Docker!
  - Run the command:

```
docker run gromacs/gromacs gmx help commands
docker run -it gromacs/gromacs
```

Demo 1: GROMACS

- An example using *pdb2gmx* from the tutorial KALP15 in DPPC:

```
$ mkdir $HOME/data ; cd $HOME/data

$ wget http://www.mdtutorials.com/gmx/membrane_protein/Files/KALP-15_princ.pdb

$ docker run -v $HOME/data:/data -w /data -it gromacs/gromacs gmx pdb2gmx -f
KALP-15_princ.pdb -o KALP-15_processed.gro -ignh -ter -water spc
```

- When prompted, choose the GROMOS96 53A6 parameter set (13) and choose "None" for the termini

Docker Image/Container Commands

Container Commands	
`docker container ls`	List docker containers currently running:

`docker container rm <container>`
`docker rm <container>`
	Remove (an) container(s):

`docker container prune`	Remove all stopped containers

Image Commands	
`docker image ls`	List docker images stored in cache:

`docker image rm <image>`
`docker rmi <image>`
	Remove (an) image(s):

`docker image prune`	Remove unused images

Docker Image/Container 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*

DockerHub

- The place where containers live! I.e. Image Registry
- Dockerhub is a Docker hosted library of public and private Docker images, with an account:
    - Free and unlimited public images
    - 1 free private repository
- Great for hosting images for fellow researchers
- "Git-like" commands

Building a Docker Container

- To build a docker container, we need a set of instructions Docker can use to set up the environment.
  - Dockerfile (<- must have this name, no extensions)
- Once we set up our Dockerfile we can use the command

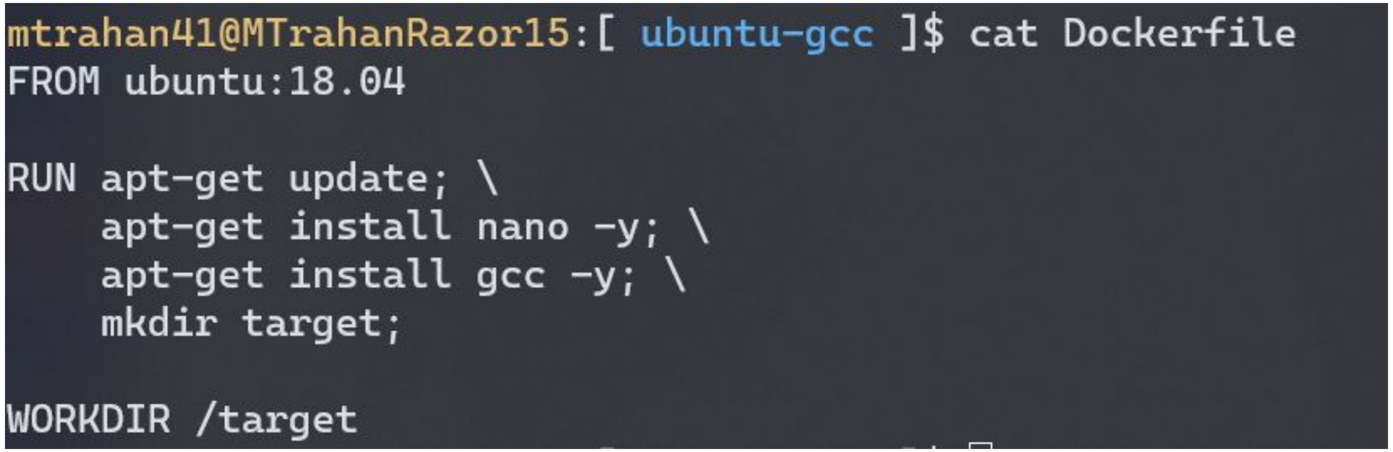
```
docker build -t <image-name> .
```

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

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

What's in a Dockerfile

- A Dockerfile is simply a text file that contains instructions to build and setup a default Image
  - Commands to build
  - Setting commands
- Requires a source Image
  - a “template” image



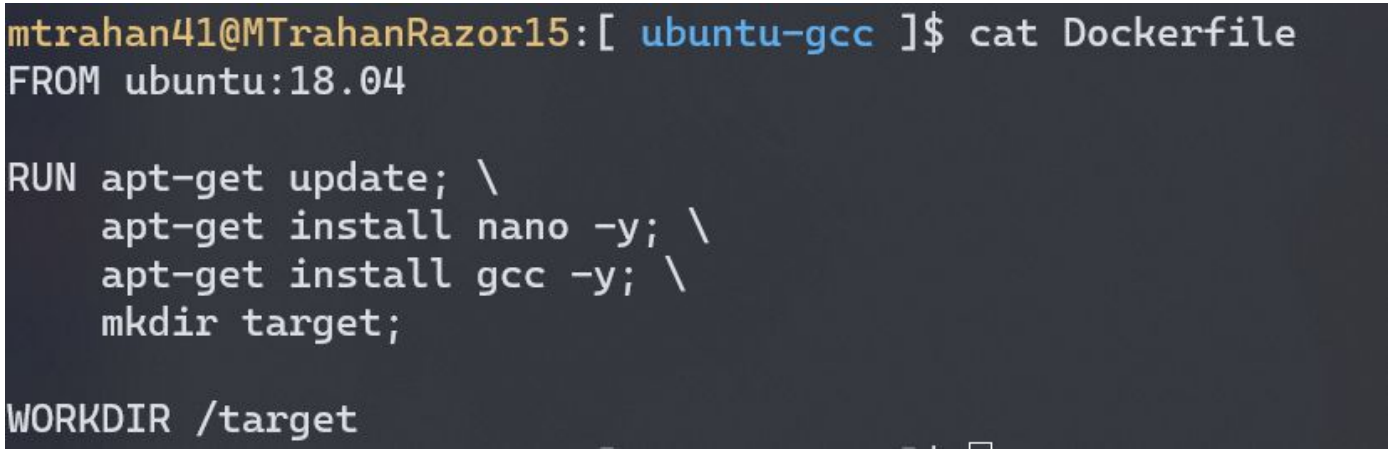
```
mtrahan41@MTrahanRazor15:[ ubuntu-gcc ]$ cat Dockerfile
FROM ubuntu:18.04

RUN apt-get update; \
    apt-get install nano -y; \
    apt-get install gcc -y; \
    mkdir target;

WORKDIR /target
```

What's in a Dockerfile

- **FROM**
  - start **FROM** a “template” image
  - base image gets pulled down from cloud
- **RUN**
  - to **RUN** terminal commands
  - install dependencies
- **WORKDIR**, **ENV**, etc…
- **CMD**
  - execute a default **CMD**



```
mtrahan41@MTrahanRazor15:[ ubuntu-gcc ]$ cat Dockerfile
FROM ubuntu:18.04

RUN apt-get update; \
    apt-get install nano -y; \
    apt-get install gcc -y; \
    mkdir target;

WORKDIR /target
```

Demo 2: Building a Docker Image

Demo 2: Ubuntu w/ GCC

- For this first example we will build 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_ROOT/dockerdemo/ubuntu-gcc
     ```
  2. Build the image with:
     ```
     docker build -t test-gcc .
     ```
- Run image as container:
  ```
  docker run -it test-gcc
  ```

Demo 2: Ubuntu w/ GCC

- What happens if we create a file in the container?

- Does it persist if we exit?
    - No! Containers are ephemeral and run in host memory

- How can we persist data?

Mounting and File Access (1)

- 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*
      - **<u>Source Directory</u>**: Directory on the host system. Never within a container.
      - **<u>Target Directory</u>**: Directory in the Docker Container. Never on the host system.
    - A flag set within the docker run command:

```
docker run -v <source-dir>:<target-dir> <image>
```

Mounting and File Access (2)

- 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 -v <volume-name>:<target-dir> <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 -v $(pwd)/source:/target test-gcc
```

- Command:

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

Modifying a Docker Image

- Suppose you have an existing docker image and want to make changes…
  - Rebuild Dockerfile!
  - Usually a bit cumbersome
- No Dockerfile? Use docker commit!
  - First you can run an image interactively and install what you need:

    ```
    $ docker run -it <image-name> bash # or any shell…
    $ apt-get update
    $ apt-get install vim
    ```
  - Exit, then commit it to a new image

    ```
    $ docker commit <container-id> <new-image-name>
    ```

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>
    ```

Demo 3: NCL container

Demo 3: NCL Container

- For this next example we will be building a Docker image that will run the NCAR Command Language (NCL)
- Dockerfile provided
- Same process:

1. Navigate to the Dockerfile found at:

```
$ CONTAINER_ROOT/dockerdemo/ncl
```

2. Build the Dockerfile and name the image: "ncl-demo"
3. Run "ncl-demo"

- Can we test a sample script?

```
$ docker run -v $(pwd)/source:/target ncl-demo ncl test.ncl
```

Docker Compose

- External 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 but comes bundled with Docker Desktop!

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>
```

- Example (after build):

```
$ docker-compose up
```

Demo 4: Docker Compose (python)

Questions?

Additional Resources

- Docker: https://www.docker.com/
- Docker Docs: https://docs.docker.com/
- Docker Hub: https://hub.docker.com/

Thank you!

- Please fill out the survey: http://tinyurl.com/curc-survey18
- Contact information: rc-help@Colorado.edu
- Slides: https://github.com/ResearchComputing/Containers_Spring_2022