Enabling Reproducibility with Docker

Research Computing
UNIVERSITY OF COLORADO **BOULDER**

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Enabling Reproducibility with Docker

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- Slides available for download at: *https://github.com/CU-Boulder-CRDDS/data_bootcamp*

Outline

- Reproducibility
- Containers
- Docker
  - Images and Containers
  - Commands
  - File Access
  - Building Docker Images
  - Dockerhub

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  - Very outdated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 its often desired for a software to be repeatable and accurate.
- *But installs are only done once. Why should I care about reproducible applications.*

The Case for Reproducibility

- 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 a packaged bundle of OS, libraries, software 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
  - Like 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
- The most common application is in Hardware Virtualization
  - Virtual Machines
    - Partitions off Memory, CPU, GPU, and Storage
    - Runs a virtual OS
    - Runs software on the virtualized machine
  - Examples: VMware, Virtualbox

Virtualization (2)

- Another use of virtualization is in OS Level Virtualization
  - Can run many isolated guest OS instances under a host OS
  - This virtualization is what is used by Docker and other container software.
  - Best of both worlds!
    - Isolated environments
    - No hardware partitioning

Containerization Software

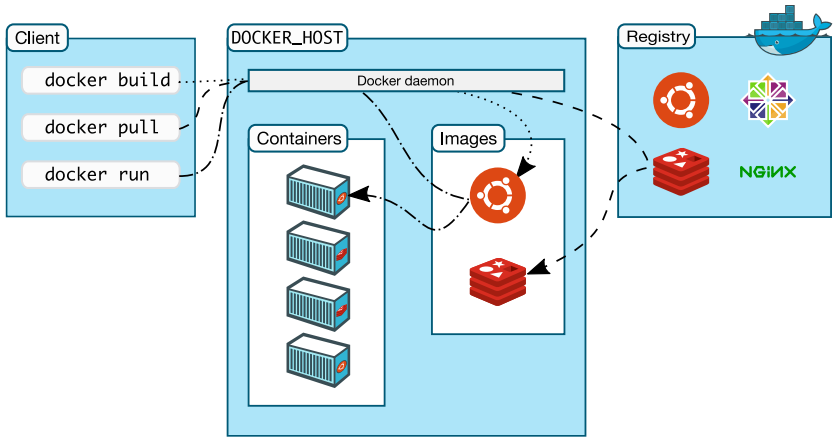
- Docker
  - Well established – largest user base
  - Has Docker Hub for container sharing
  - Problematic with HPC (Fix incoming!)
- Singularity
  - Designed for HPC
  - Second largest userbase
  - Developed for scientific use
- Charliecloud; Shifter
  - Designed for HPC
  - Based on Docker
  - Less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

Installing Docker

- Docker Community Edition
  - Comfy GUI to help keep track of containers and images!
  - Available on all operating systems
  - Windows users can enable WSL2 support following the instructions here: https://docs.docker.com/docker-for-windows/install/
- 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 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.
- Specify commands after your image to execute specific software in your container.

  docker run <image-name> <program>

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'**

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
      - 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 -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 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!

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 like 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>

Building a Docker Container

- 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 a Docker Image

Demo 2: Custom Python installation

- Lets set up a shareable Python image holding all the required packages for our workflow:
  - Python 3.9.6-slim
  - Numpy and Matplotlib
- Run an example script
- Push to Dockerhub!

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!

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

  - Then commit it to the image

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

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!

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/CU-Boulder-CRDDS/data_bootcamp