Barcelona-2023_byBpiereck

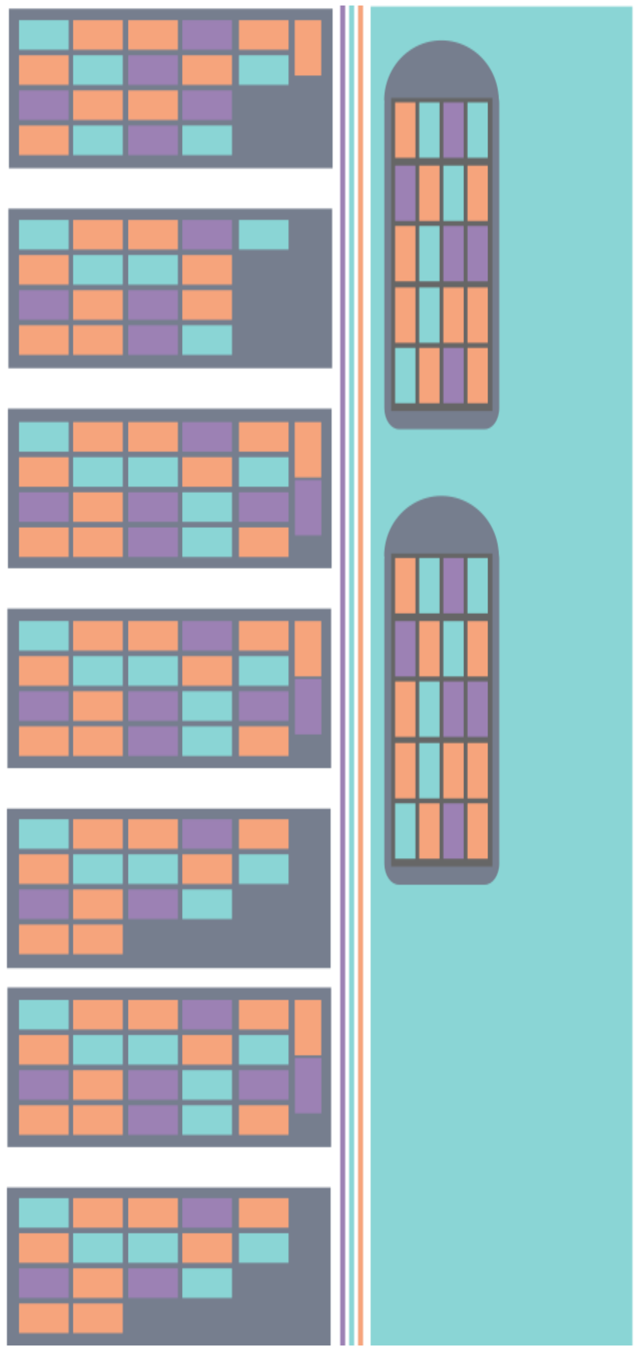
Introduction to Docker for reproducible analysis

What are CONTAINERS ?

- Common definition: Object to **HOLD** and **TRANSPORT** something

How are containers related to informatics ?

- Co-relation in informatics: It is a **PORTABLE** package **HOLDING** applications and all its necessary means.



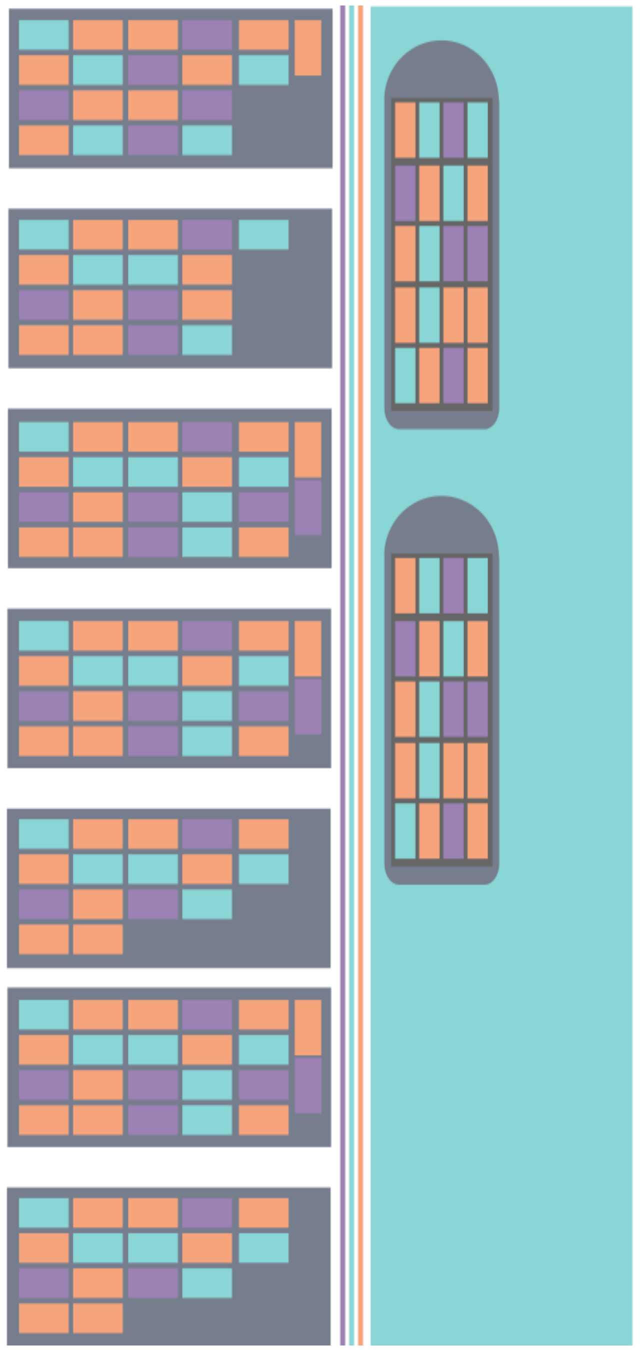
What is a DOCKER ?

- Common definition: Person working in a port, responsible for **LOADING** and **UNLOADING** containers.

How is a DOCKER related to (bio)informatics?

- Co-relation in informatics: It is an open-source platform to
  - **CREATE** (loading),
  - **MANAGE** (running)
  - **SHIP** (sharing)

  containers with their applications.

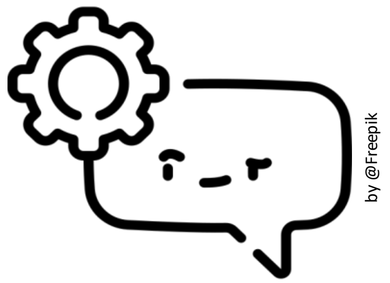


What is a container ?

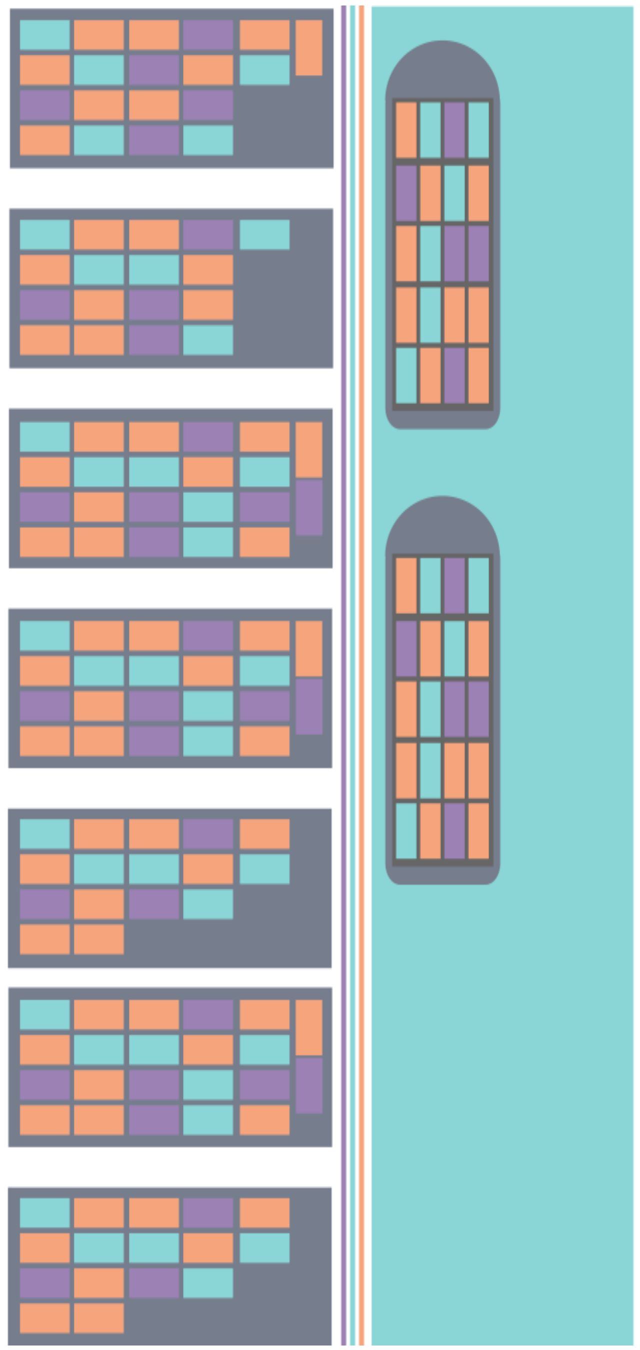
“ *A container image is a **lightweight, stand-alone, executable** package of a piece of software that **includes everything** needed to run it: code, routine, system, tools, libraries, settings* ”

- *https://www.docker.com/what-container* -

“Well, it works on my machine…”



- Potential general barriers
  - Different Operational system
  - Different hardware
  - Different software versions
  - Technical ability



Docker use cases

by @Freepik

- Web application
  - Galaxy, GitLab

by @Irfansusanto20

- Analysis pipeline
  - Nextflow, Snakemake

by @kerismaker

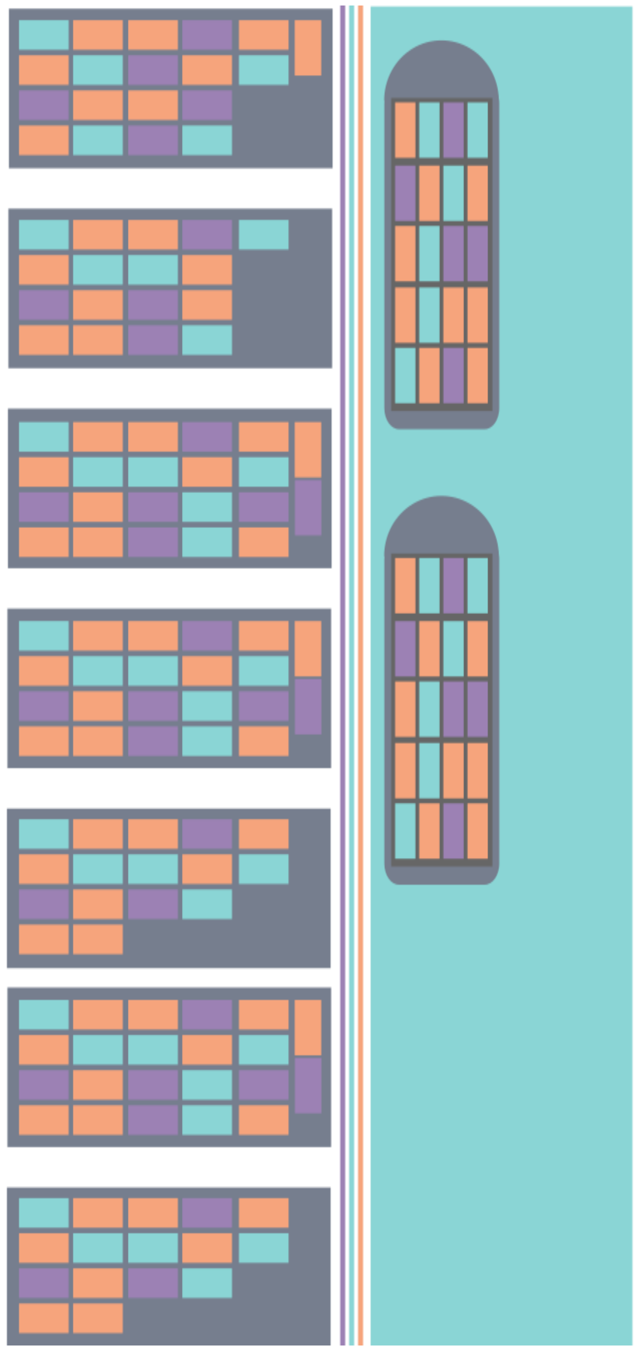
- Testing & continuous integration
  - Jenkins, Drone CI

by @Freepik

- Difficult to compile apps
  - PennCNV, hap.py

by @Creaticca Creative Agency

- Need for reproducible environments
  - Jupyter notebooks



How does it work?

- Important concepts
  - **Dockerfile:** Your recipe
  - **Docker image:** Static artifact
  - **Container:** Running image (functional)
  - **Backup.tar:** Compacted file
  - **Docker engine:** ‘Manager’

Recipe
images
containers
Backup.zip

your recipe to build
the Docker image

File you can create
using the docker engine
(rarely used)

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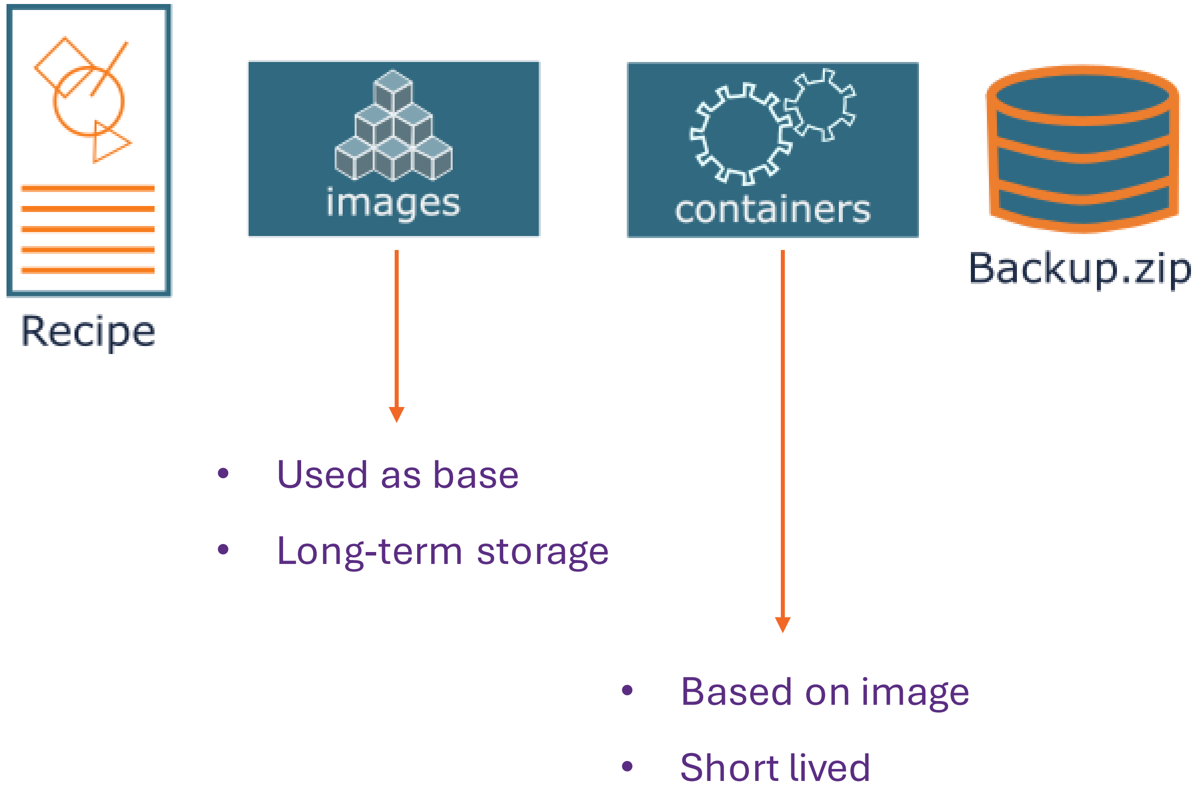

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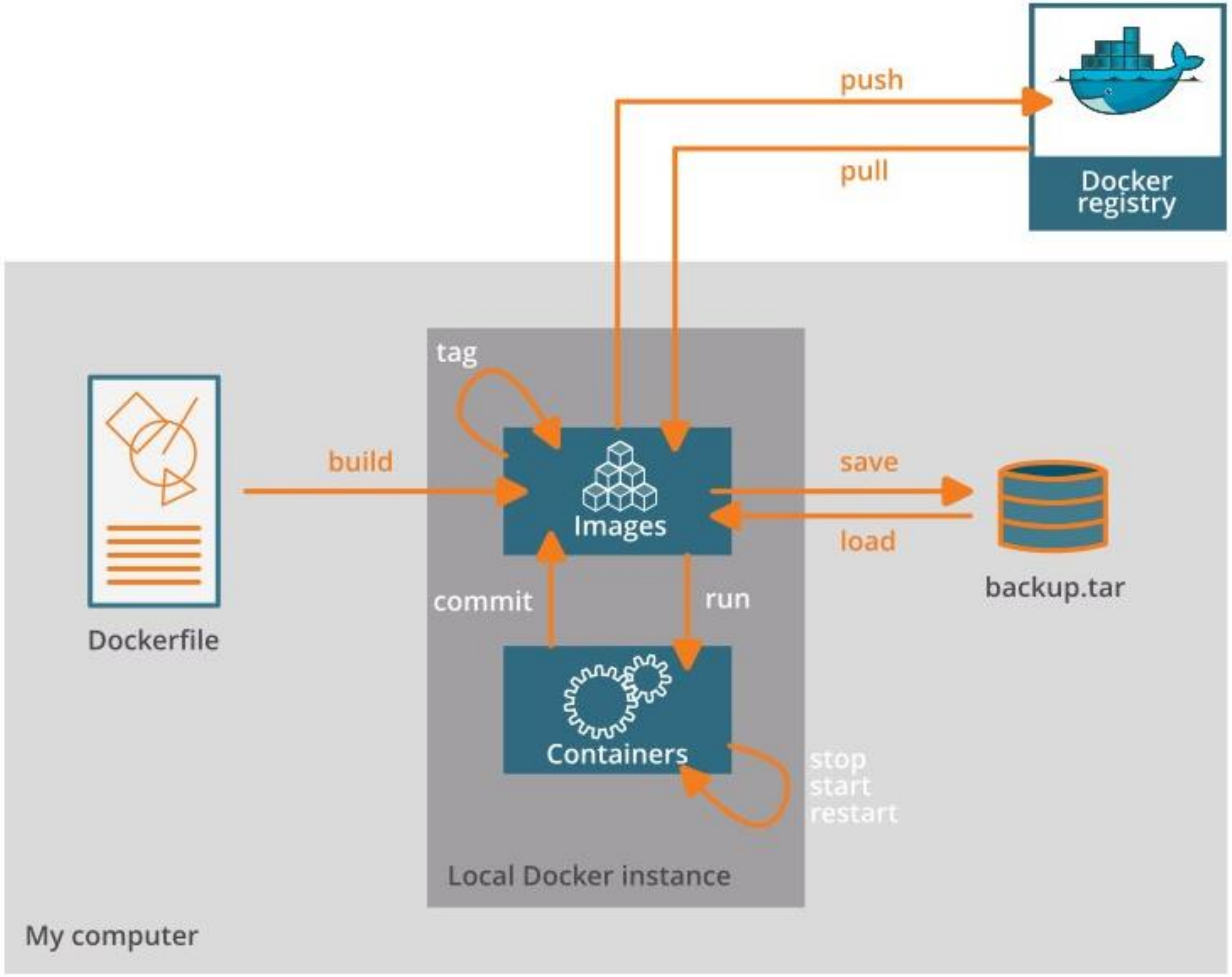

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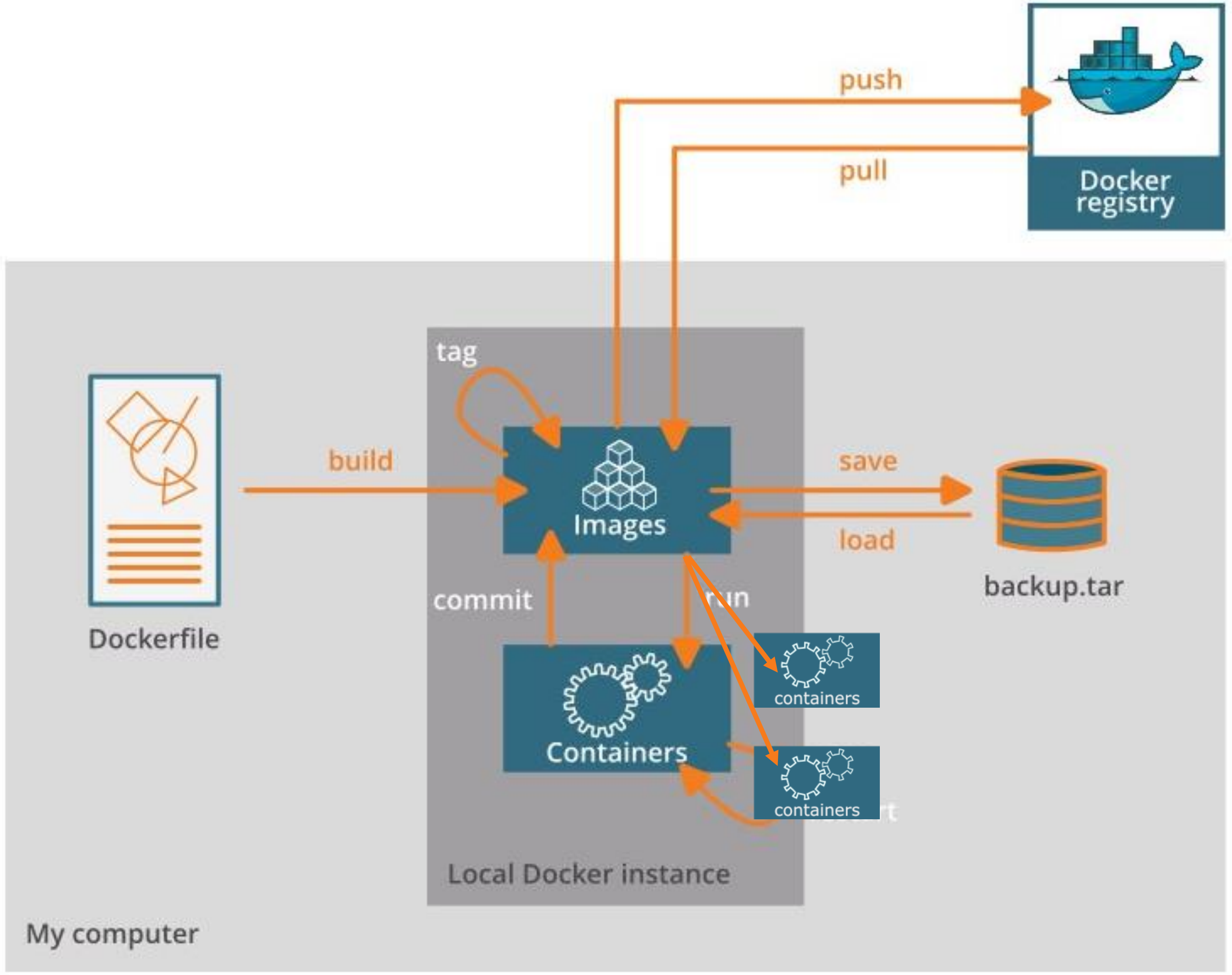


How is it organized?

- General components

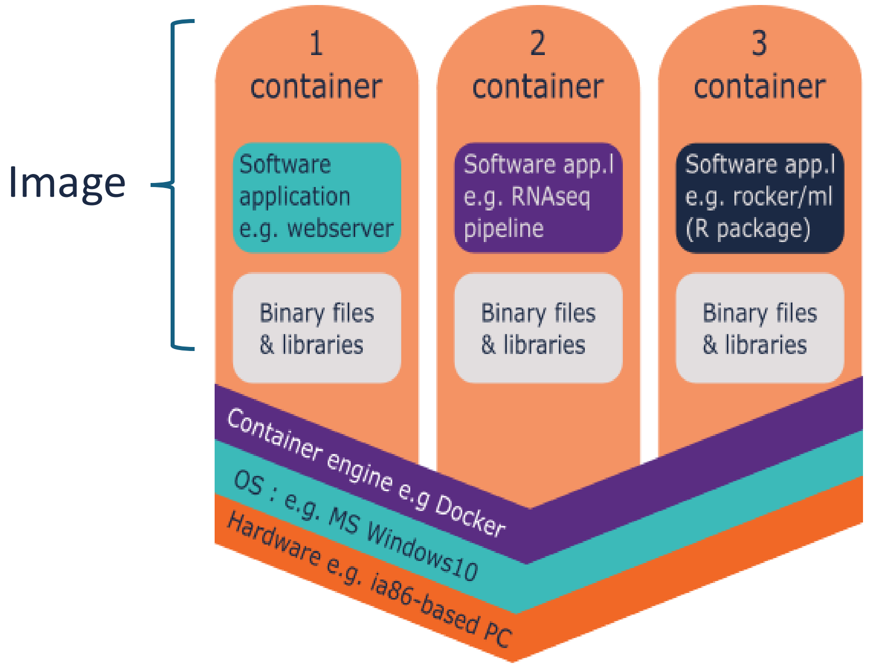
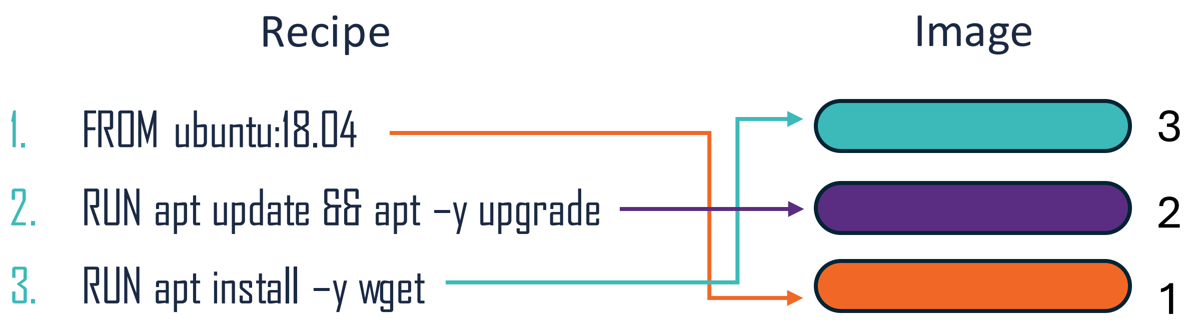


Image
1 container
2 container
3 container
Software application e.g. webserver
Software app.l e.g. RNAseq pipeline
Software app.l e.g. rocker/ml (R package)
Binary files & libraries
Binary files & libraries
Binary files & libraries
Container engine e.g Docker
OS : e.g. MS Windows10
Hardware e.g. ia86-based PC

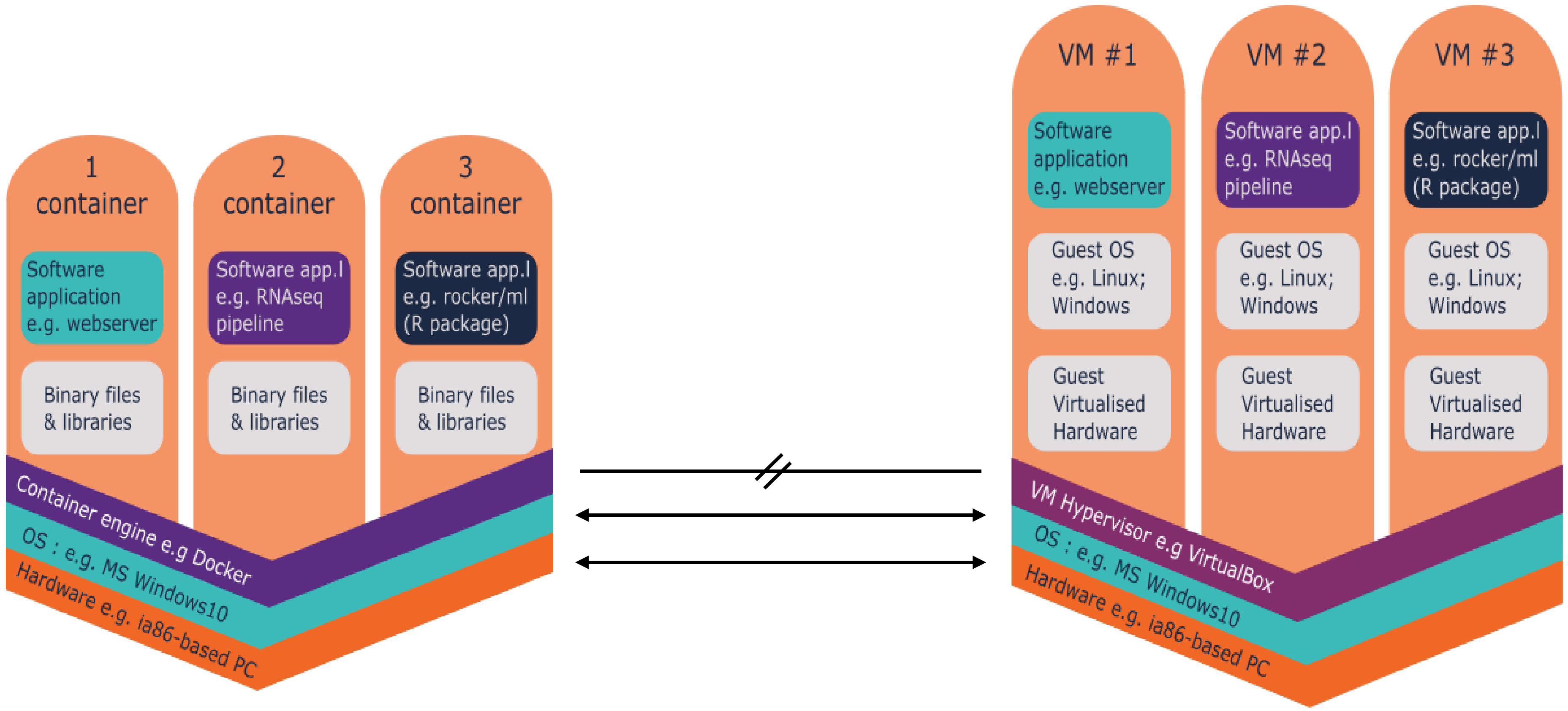
- Docker images layers



1. FROM ubuntu:18.04
2. RUN apt update && apt -y upgrade
3. RUN apt install -y wget

How is it organized?

- General components
- Docker images layers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Software application e.g. webserver
Binary files & libraries
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3 container
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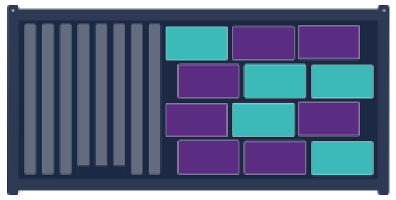
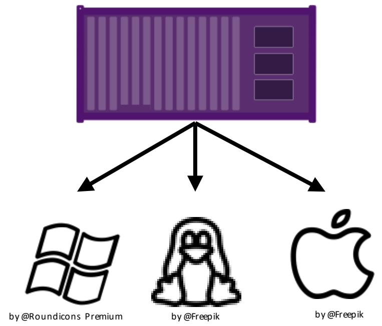
Binary files & libraries
Container engine e.g Docker
OS : e.g. MS Windows10
Hardware e.g. ia86-based PC
VM #1
Software application e.g. webserver
Guest OS e.g. Linux; Windows
Guest Virtualised Hardware
VM #2
Software app.l e.g. RNAseq pipeline
Guest OS e.g. Linux; Windows
Guest Virtualised Hardware
VM #3
Software app.l e.g. rocker/ml (R package)
Guest OS e.g. Linux; Windows
Guest Virtualised Hardware
VM Hypervisor e.g VirtualBox
OS : e.g. MS Windows10
Hardware e.g. ia86-based PC

Advantages

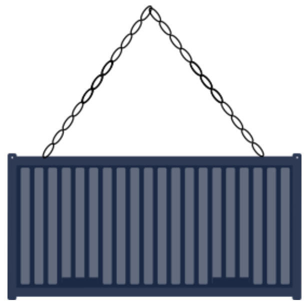
- **Bundled Dependencies**
  - Contain all their own dependencies = no need of installing hurdles



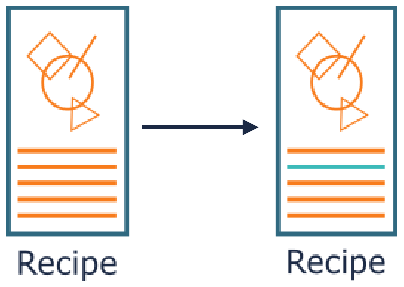
- **Cross-platform Installation**
  - Contain their own operating system = run on any platform (even Windows!)



- **Easy Distribution**
  - Shared on Docker Hub or as ‘image.tar’ file



Advantages



- **Safety**
  - Can’t access files on the host machine
- **Ease-of-Use**
  - Can always be run using one single command
- **Easy Upgrades**
  - Easily swapped out for newer versions
  - All persistent data can be retained in a data volume

Other container softwares

podman

Charliecloud

SMALL SOFTWARE DELIVERING BIG FLEXIBILITY TO HPC

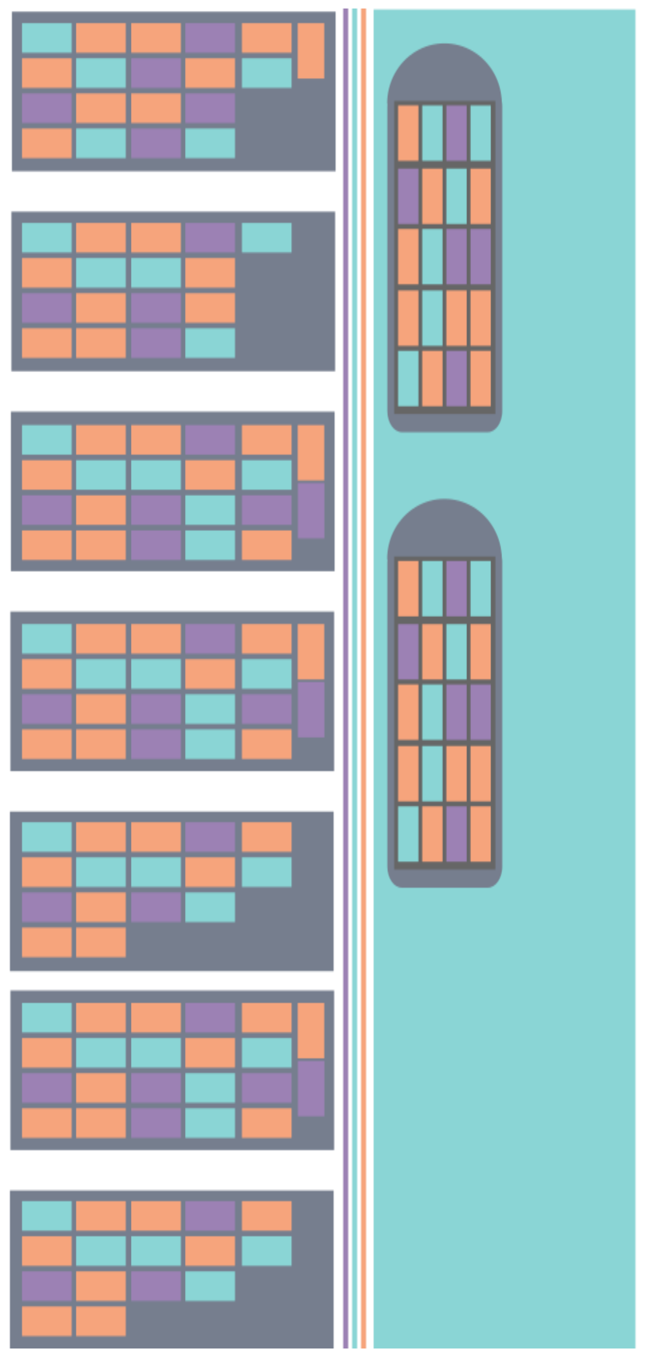
APPTAINER

Using and Reusing available docker images

Where can we storage and find Docker images?

Local storage

Registry



Where can we storage and find Docker images?

Local storage

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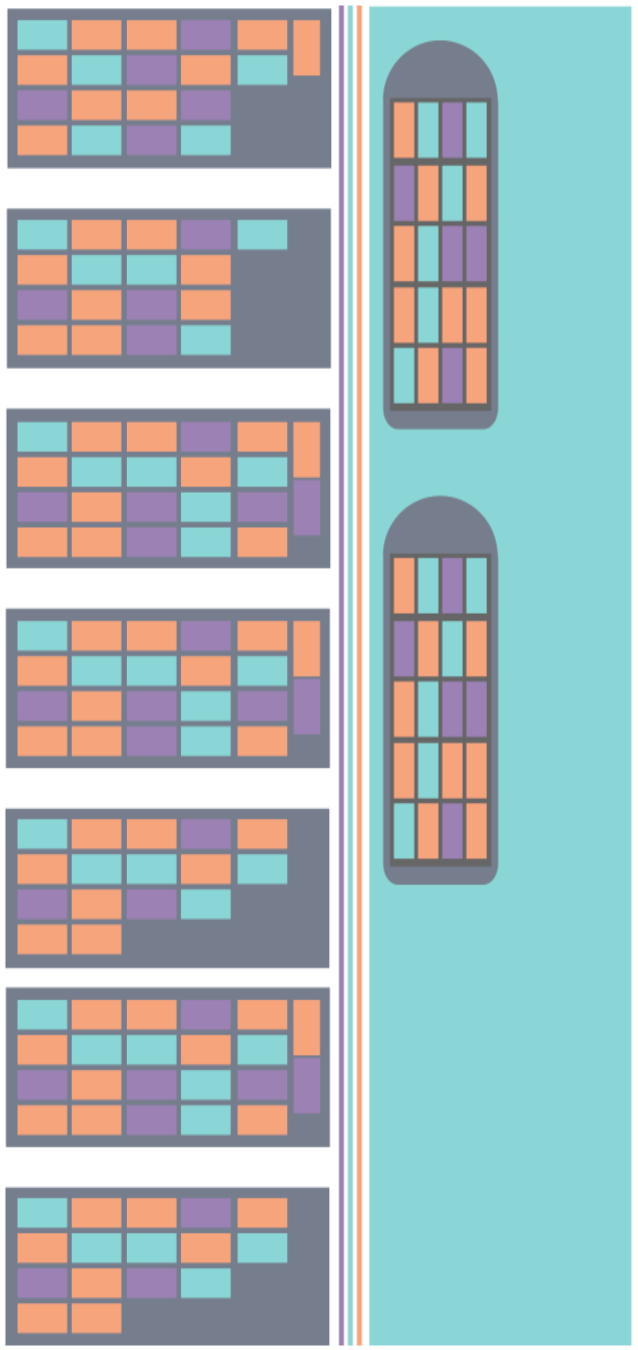
Preferable



Container Registries

- Main registry for DOCKER containers

docker hub

- Alternative registries

Azure Container Registry

QUAY

HARBOR

Google Container Registry

Gitlab Container Registry

JFrog

Amazon ECR

Container Registries

BioContainers

docker hub

QUAY

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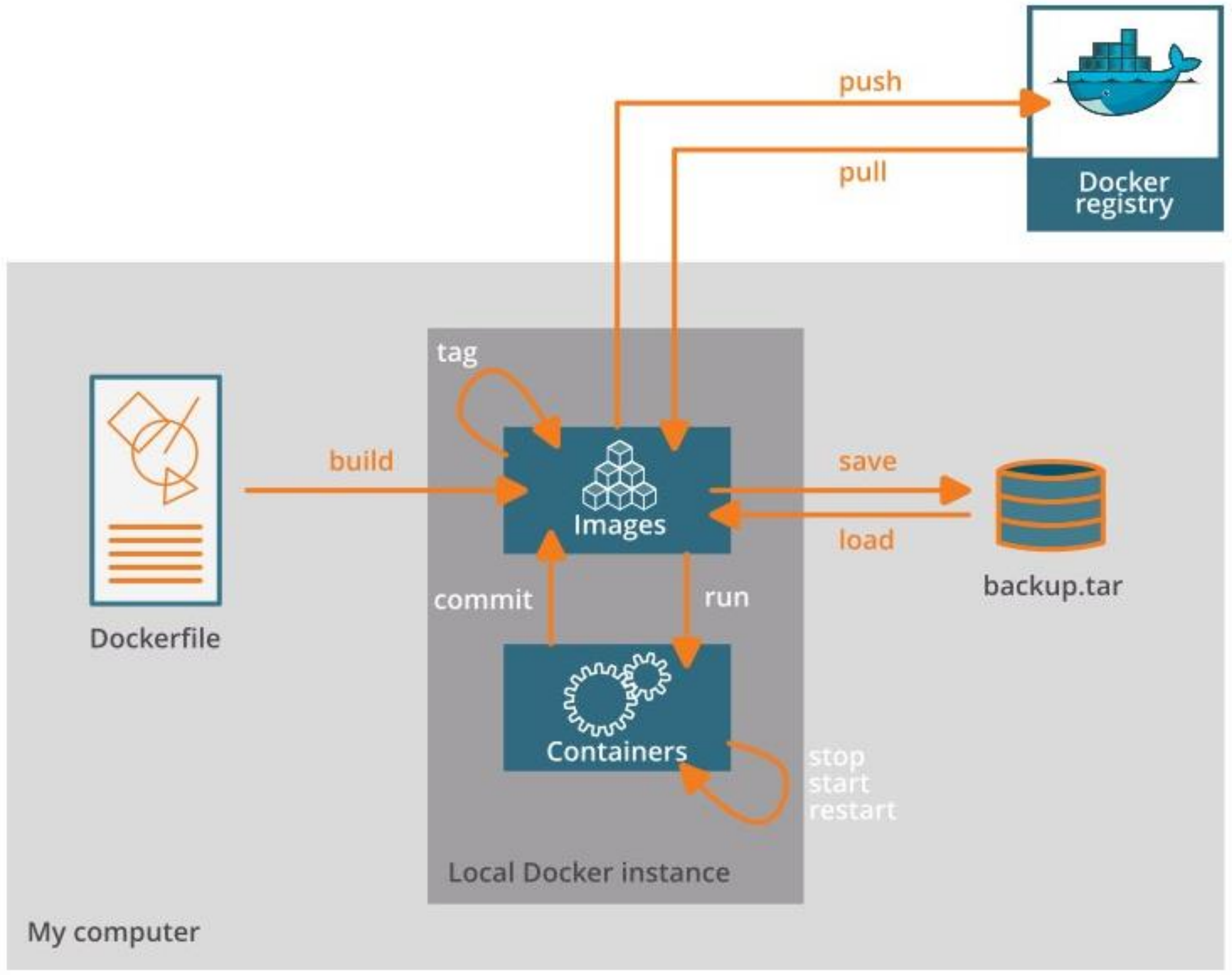
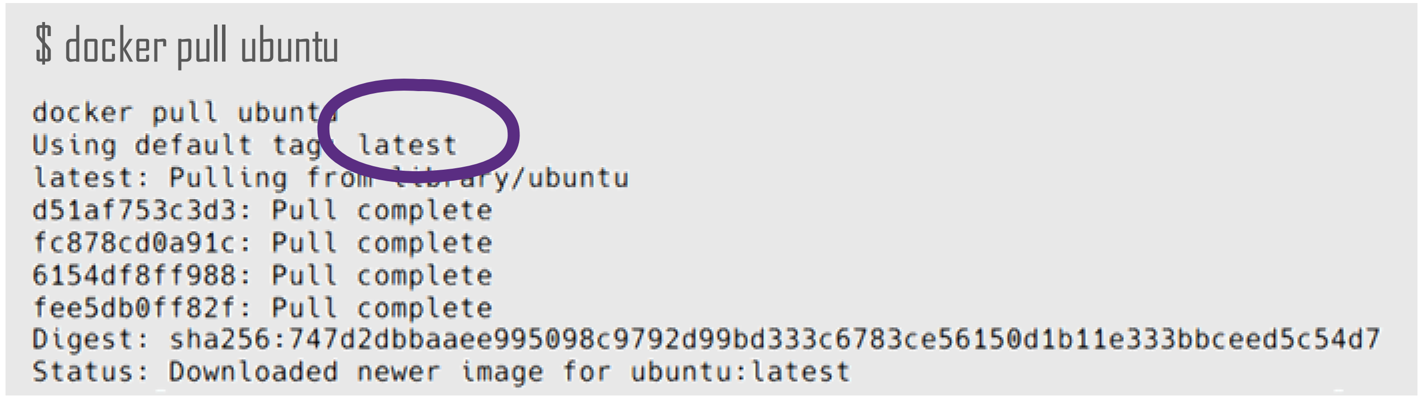
How do we get a container image?



How do we get a container image?

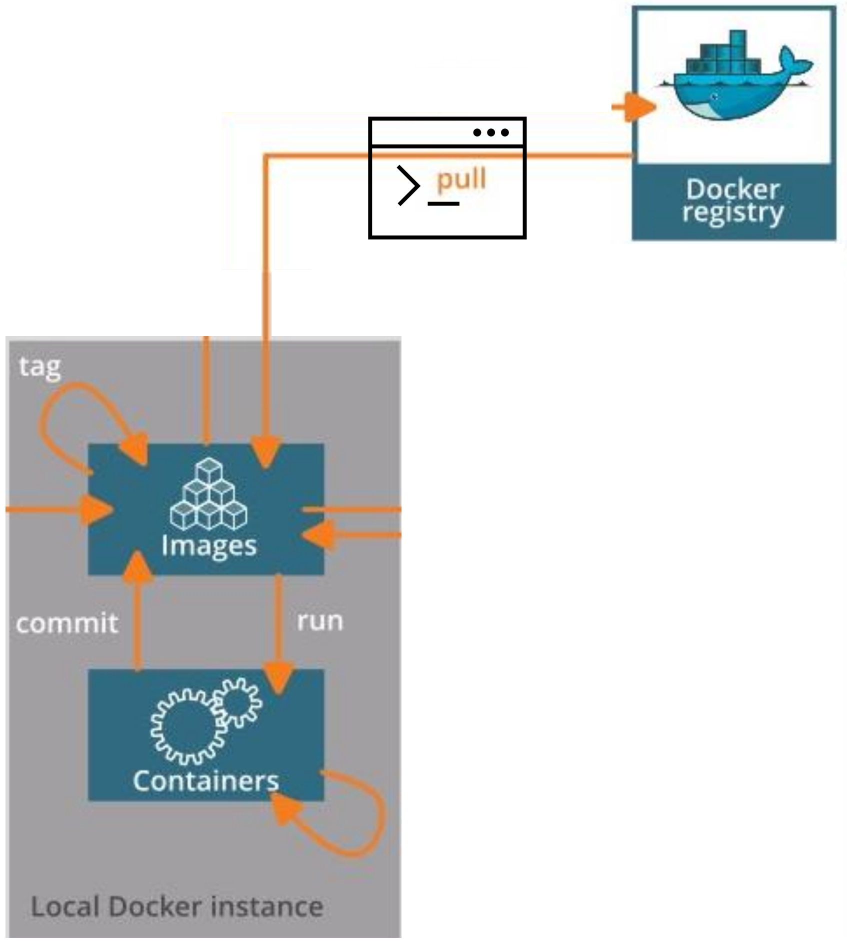
- docker pull <image>
- docker pull <registry/image>

  - Example: getting Ubuntu image



```
$ docker pull ubuntu

docker pull ubuntu
Using default tag: latest
latest: Pulling from library/ubuntu
d51af753c3d3: Pull complete
fc878cd0a91c: Pull complete
6154df8ff988: Pull complete
fee5db0ff82f: Pull complete
Digest: sha256:747d2dbbaaee995098c9792d99bd333c6783ce56150d1b11e333bbceed5c54d7
Status: Downloaded newer image for ubuntu:latest
```



How do we get a container image?

- docker pull <image>
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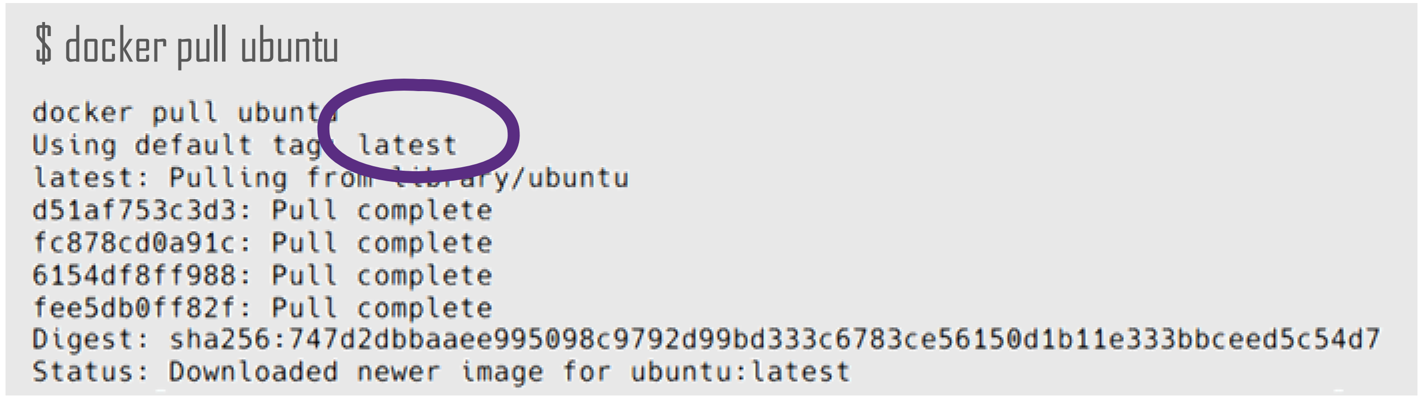
  - Example: getting Ubuntu image



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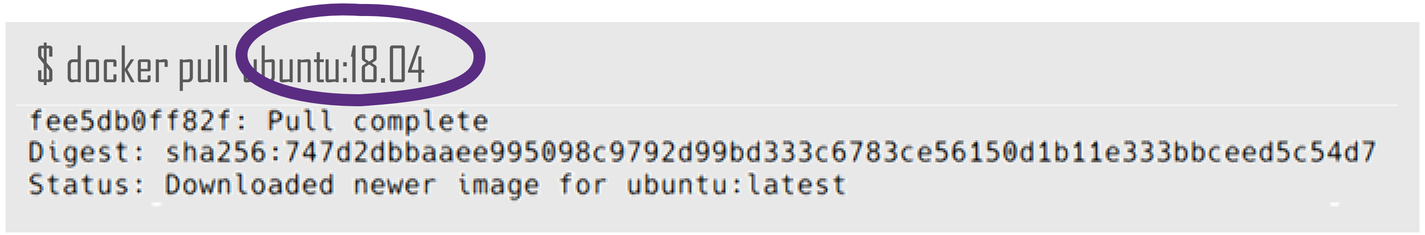
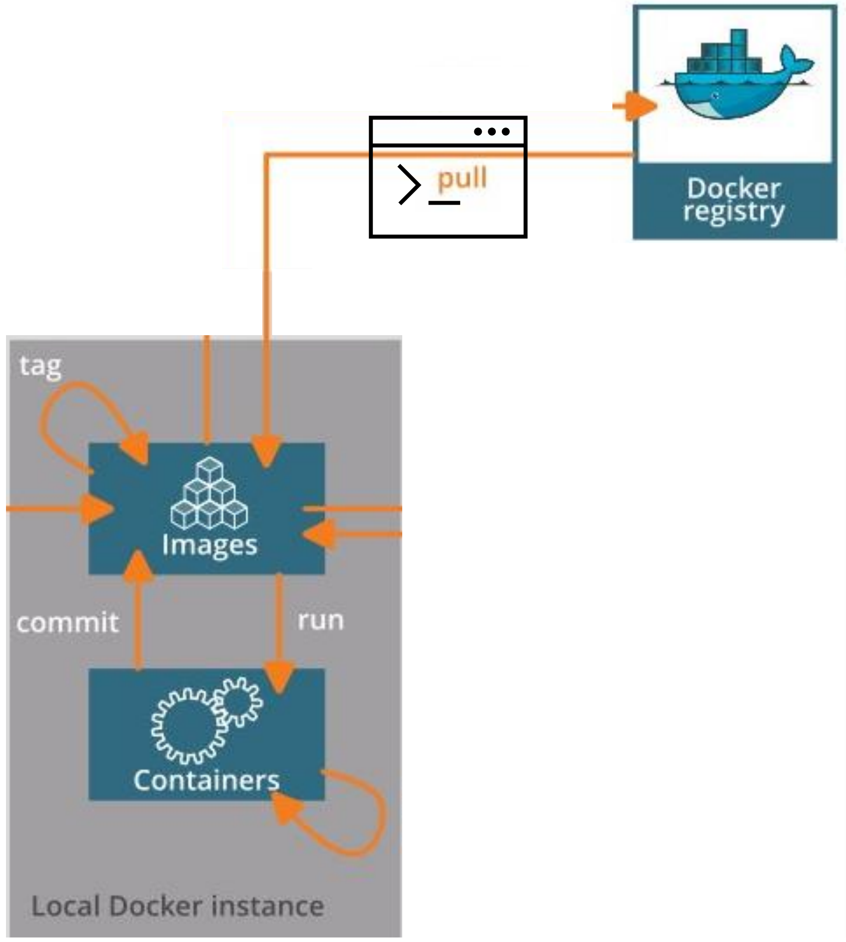
Digest: sha256:747d2dbbaaee995098c9792d99bd333c6783ce56150d1b11e333bbceed5c54d7
Status: Downloaded newer image for ubuntu:latest
```

  - Example: Get a specific version

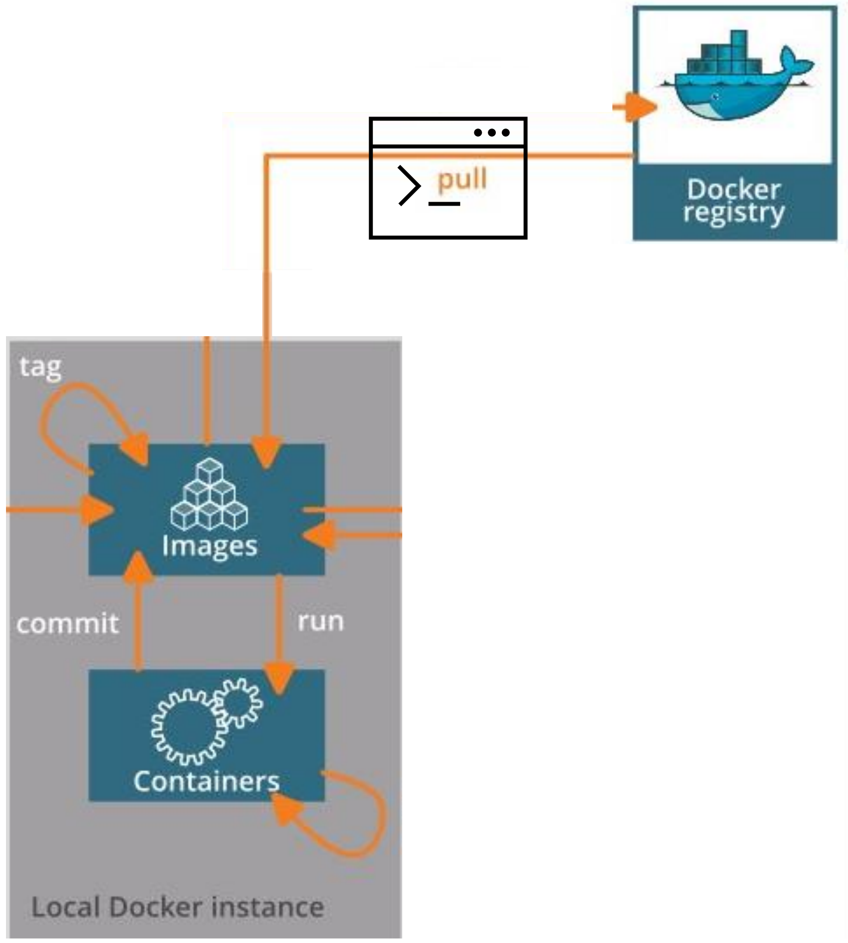


```
$ docker pull ubuntu:18.04
fee5db0ff82f: Pull complete
Digest: sha256:747d2dbbaaee995098c9792d99bd333c6783ce56150d1b11e333bbceed5c54d7
Status: Downloaded newer image for ubuntu:latest
```



QUIZ TIME: How do we get a container image?

- Is there a better way to 'pull' ??
- If yes, which one?
  - docker pull ubuntu
  - docker pull ubuntu:18.04
- Why?



Practice time: How do we get a container image?

- Pull ubuntu in your computer:
  - Version 18.04

- Pull from Biocontainers
  - Fastqc (A quality control tool for high throughput sequence data)
  - Version 0.11.9_cv7

What else can we do?

- Check all images that you have

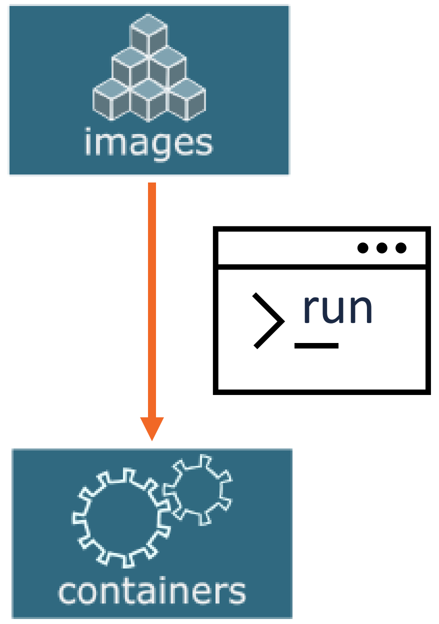
```
$ docker images
```

```
$ docker image ls
```

```
$ docker images -a
```

- Run a container with your analysis

```
$ docker run [docker_options] <container> [container_arguments]
```



Practice time: List your imaged

- List all the images you have pulled or build

Practice time: Run your 1st image

- List all the images you have pulled or build

You can execute any program/command that is stored inside the image.

- Run your 1st container

```
$ docker run ubuntu:18.04 /bin/ls

$ docker rum ubuntu:18.04 /bin/whoami

$ docker run ubunu:18.04 /
```

Practice time: Run your 1st image

- List all the images you have pulled or build

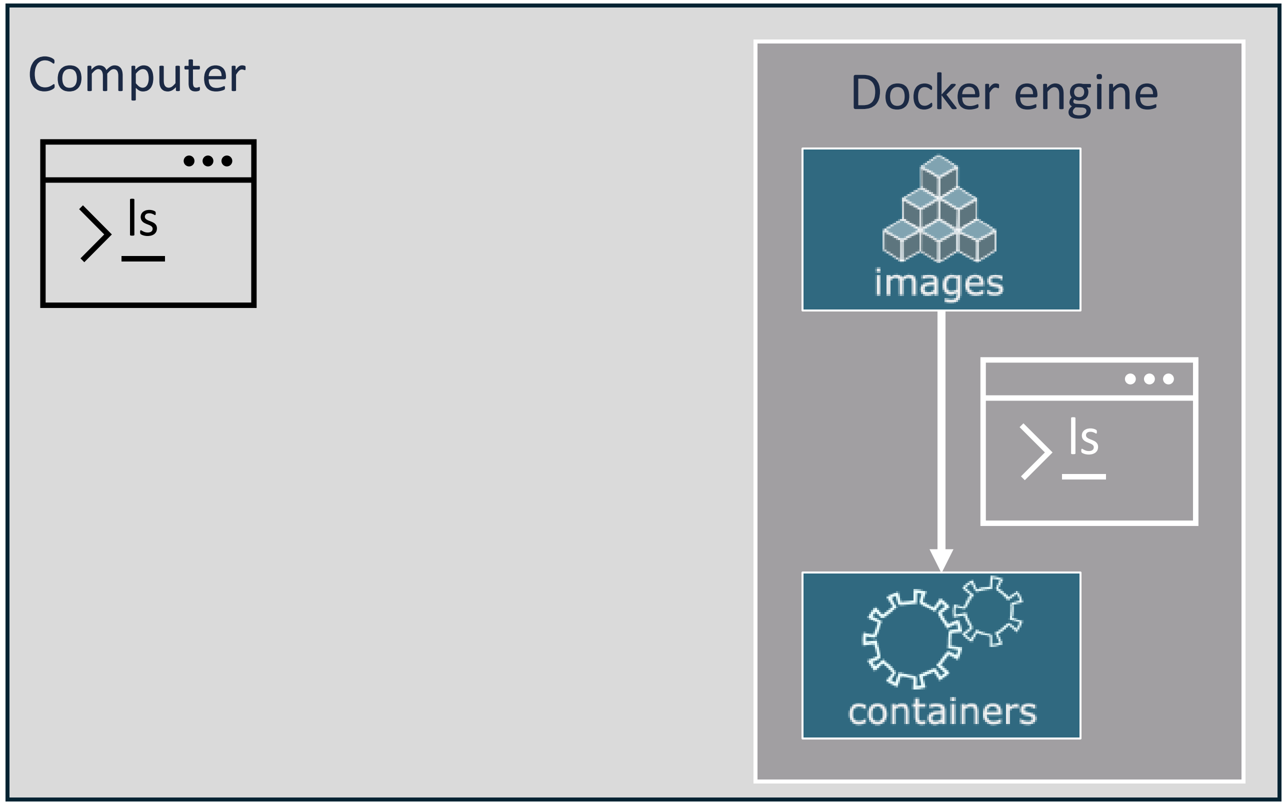
You can execute any program/command that is stored inside the image.

- Run your 1st container

```
$ docker run ubuntu:18.04 /bin/ls
```

- If you run `ls` in your current directory, do you have the same?

- Why?



Docker detach, what does It do?

Docker detach, what does It do?

- Run in the background
  - Detached from the shell

```
$ docker run [docker_options] <container> [container_arguments]
```

```
$ docker run --detach <container> [container_arguments]
```

- Name your container to check later

```
$ docker run --detach --name <my_ctn_name> <container> [container_arguments]
```

Practice time:

- Run the following without naming it:

```
$ docker run --detach nginx
```

- Run again naming it

```
$ docker run --detach --name MyUbuntu nginx
```

Challenge: How do you list running containers?

Practice time:

- Run the following without naming it:

```
$ docker run --detach nginx
```

- Run again naming it

```
$ docker run --detach –name MyUbuntu nginx
```

-

Challenge: How do you list running containers?

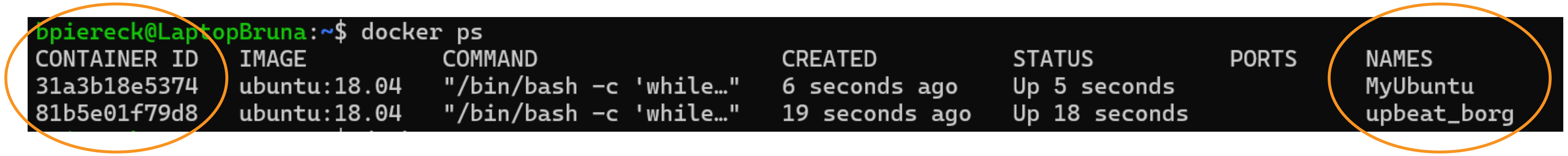
- List running containers

```
$ docker ps
```

- List all containers (whether or not running)

```
$ docker ps -a
```

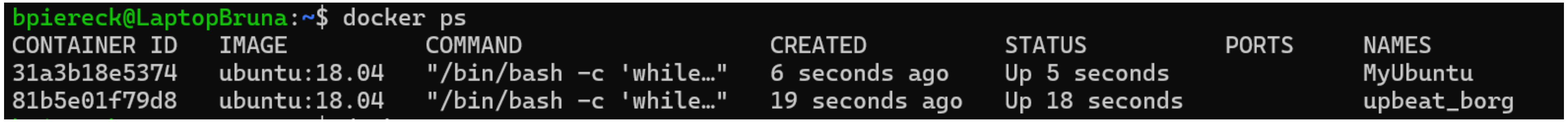
Practice time:



```
bpiereck@LaptopBruna:~$ docker ps
CONTAINER ID   IMAGE          COMMAND                  CREATED          STATUS          PORTS     NAMES
31a3b18e5374   ubuntu:18.04   "/bin/bash -c 'while…"   6 seconds ago    Up 5 seconds              MyUbuntu
81b5e01f79d8   ubuntu:18.04   "/bin/bash -c 'while…"   19 seconds ago   Up 18 seconds             upbeat_borg
```

- What are IDs and Names useful for?

Practice time:



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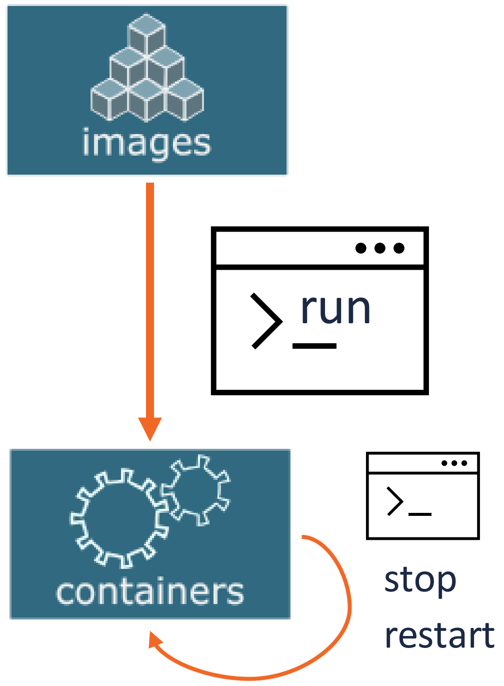
```

- What are IDs and Names useful for?
  - Stop a container
  - Restart a container



Tagging

- Name your image!
  - Version of your image

```
docker tag <image ID> <tag_name>
```

Let’s try to do it!

Tagging

- Name your image!
    - Version of your image

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docker tag <image ID> <tag_name>
```

Let’s try to do it!

- Check the ID of your images
- Chose one of them to change or add a tag

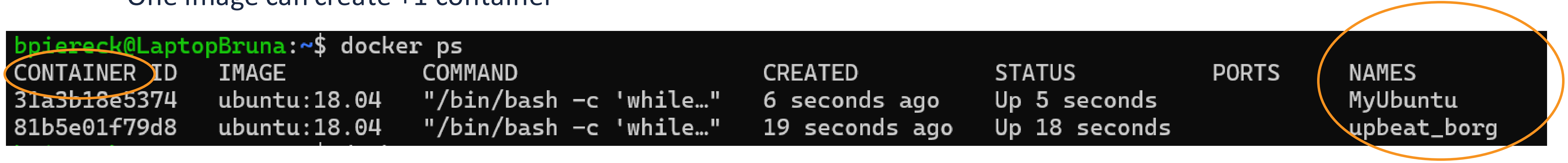
QUIZ TIME: Naming objects in Docker

- What is the difference between … ?
  - Tag
  - --name

QUIZ TIME: Naming objects in Docker

- What is the difference between … ?
  - Tag
  - --name

- Name the container (docker run –name ….)
  - One image can create +1 container



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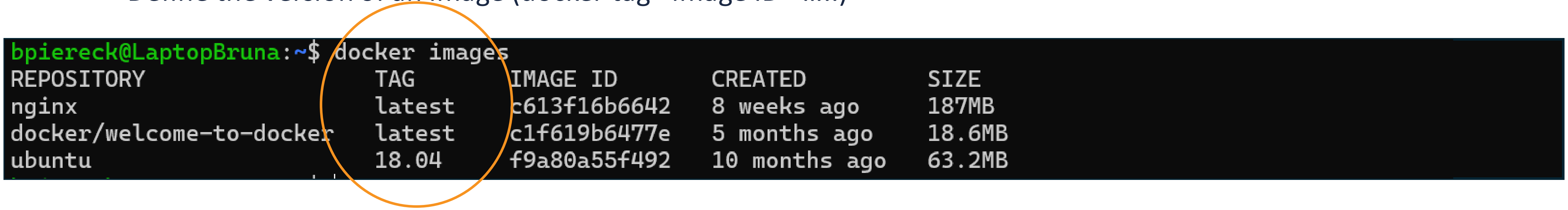
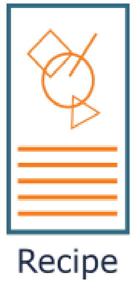
- Name an image
  - Define the version of an image (docker tag <image ID> …..)



```
bpiereck@LaptopBruna:~$ docker images
REPOSITORY                 TAG       IMAGE ID       CREATED          SIZE
nginx                      latest    c613f16b6642   8 weeks ago      187MB
docker/welcome-to-docker   latest    c1f619b6477e   5 months ago     18.6MB
ubuntu                     18.04     f9a80a55f492   10 months ago    63.2MB
```

Docker and disk space

- Docker objects are not automatically removed
  - Images
  - Containers
  - Networks
  - Volumes
- Check system space
- Pruning the system
  - The whole system
  - Dangling images
    - Not tagged
    - No references
  - All images not associated to a container



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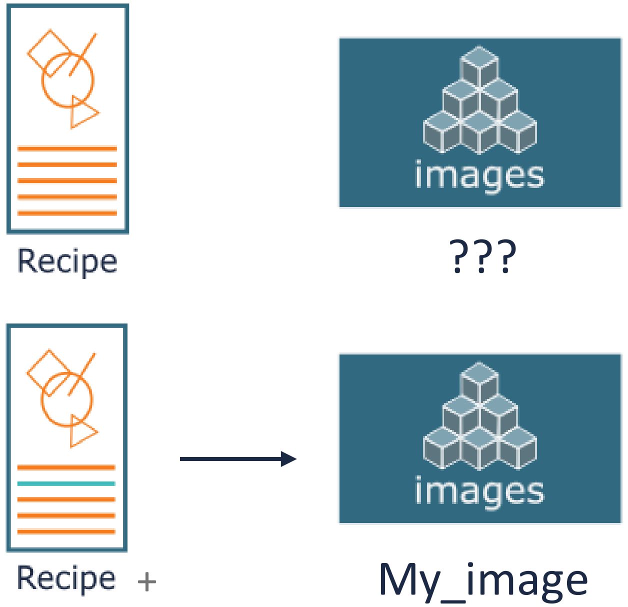

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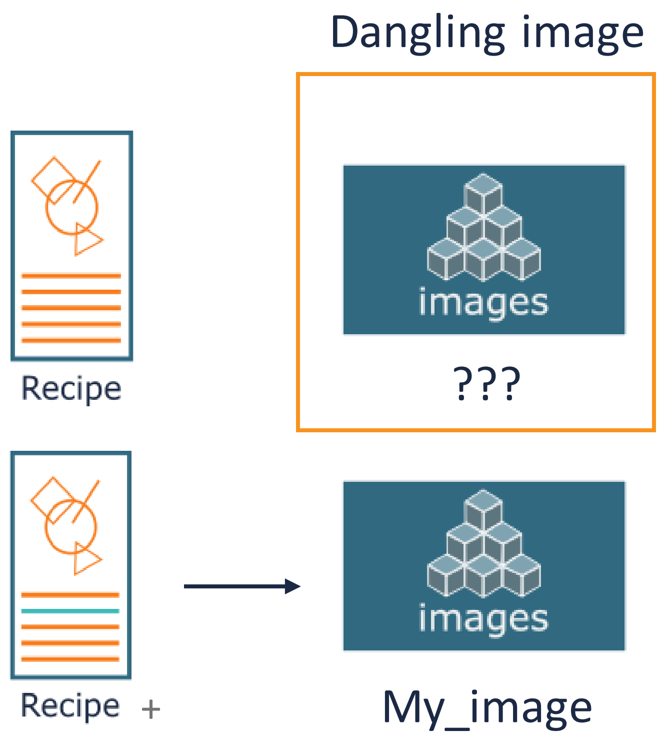

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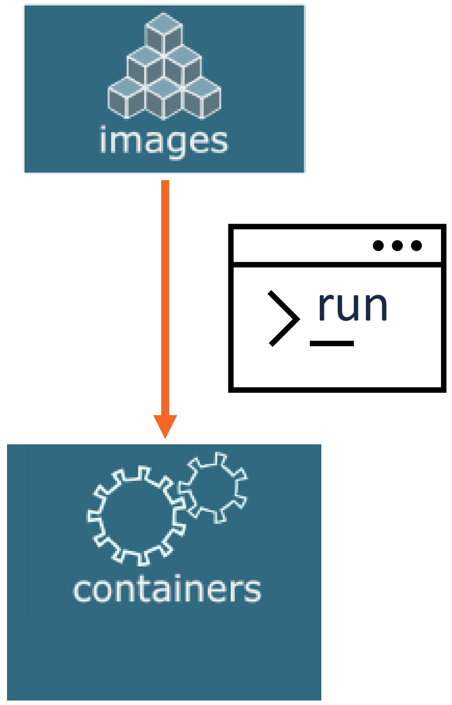

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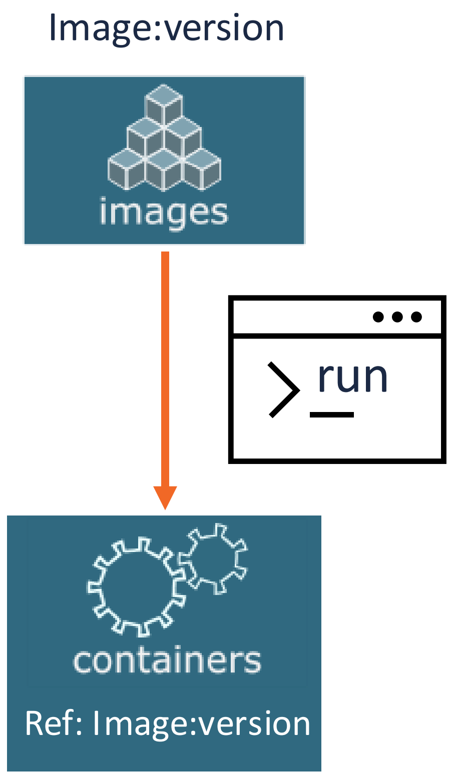

Docker and disk space

- Check space usage (**D**isk in**F**o)
  - Output
    - Type object
    - Total number of objects
    - Size
    - etc

```
$ docker system df
```

Docker and disk space

- Check space usage (**D**isk in**F**o)
  - Output
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```
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```

- Clean up
  - Remove (rm)
    - Specify
      - Image
      - Container

```
$ docker rm –f <container>
```

```
$ docker rmi <image>
```

Docker and disk space

- Check space usage (**D**isk in**F**o)
  - Output
    - Type object
    - Total number of objects
    - Size
    - etc

```
$ docker system df
```

- Clean up
  - Remove (rm)
    - Specify
      - Image
      - Container

```
$ docker rm  <container>
```

```
$ docker rmi <image>
```

  - Major clean up
    - Clean all dangling objects
    - $ docker system prune
    - Clean all dangling images

```
$ docker image prune
```

    - Clean unused containers

```
$ docker container prune
```

Docker and disk space

- Check space usage (**D**isk in**F**o)
  - Output
    - Type object
    - Total number of objects
    - Size
    - etc

```
$ docker system df
```

Clean all UNUSED objects

```
$ docker system prune –a
```

Use it carefully !!!

- Clean up
  - Remove (rm)
    - Specify
      - Image
      - Container

```
$ docker rm –f <container>
```

```
$ docker rmi <container>
```

- Major clean up
  - Clean all dangling objects

```
$ docker system prune
```

  - Clean all dangling images

```
$ docker image prune
```

  - Clean unused containers

```
$ docker container prune
```

Practice time: Check and clean

- Check how much disk space you've used
- Clean stopped or unused containers
- Can you combine docker options?
  - run
  - rm
  - prune
  - tag

Working interactively

- When to do it?
  - Debug
- How to do it:
  - docker run –it <image> <command>
  - dokcer run –it –rm <image> <command>
  - dockcer exec <containerr>

ACTIVITY TIME:

- Activity 1.1
  - Get the data (https://github.com/vibbits/containers-workshop/)
  - You will need fastqc
    - check all your images
    - Pull image if needed
  - Run fastqc –h

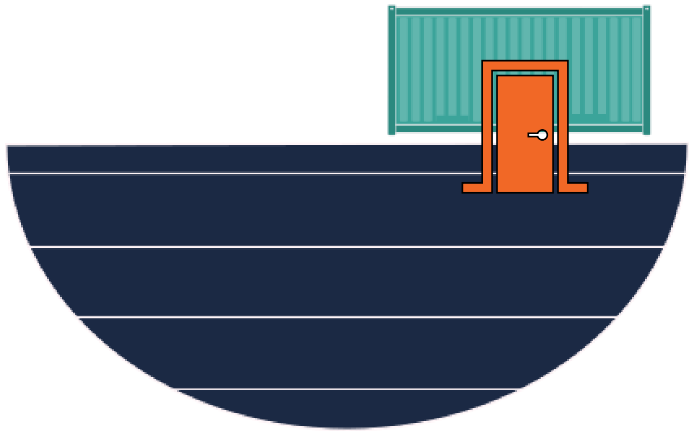
- Activity 1.2
  - Check for running containers
  - Remove the container
  - Run the container interactively
    - Start it with bash

Docker a closed environment

Docker a closed environment

- Mounting volumes

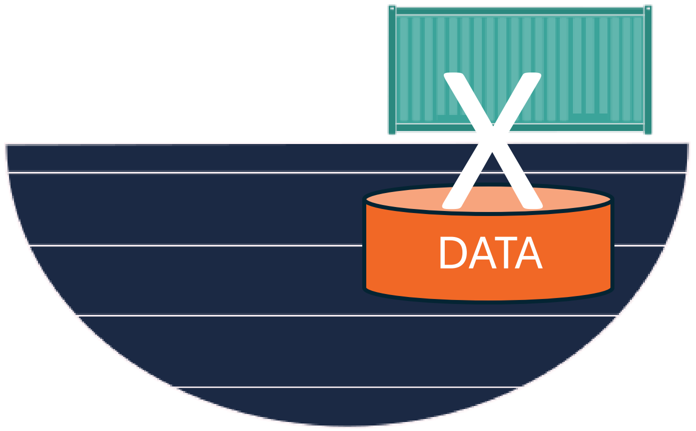
- Using Ports



Volume mounting: I/O

- Activity 2 -3 and 4.1

- Container is isolated from host



Volume mounting: I/O

- Container is isolated from host
- Data in the container is NOT kept

- Activity 2 -3 and 4.1

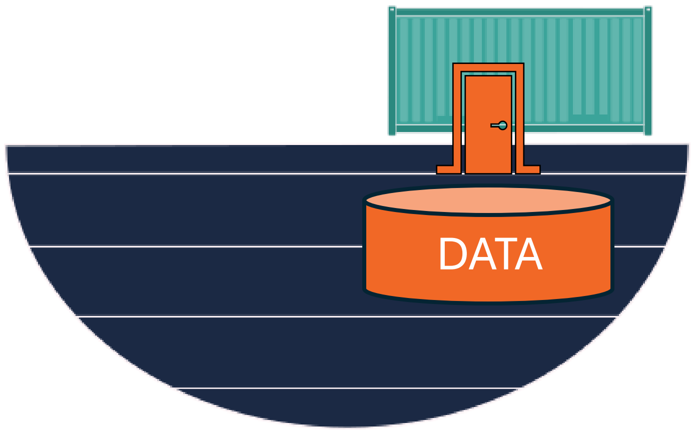
Volume mounting: I/O

- Activity 2 -3 and 4.1

- Container is isolated from host
- Data in the container is NOT kept
- Solution:
    - Biding volume

-v /path/in/host:/path/in/container

```
docker run --detach \
--volume path/in/host/datatest:/path/in/container/dataset \
--name <container_name><container:version><container_options>
```



Volume mounting: I/O

- Activity 2 -3 and 4.1

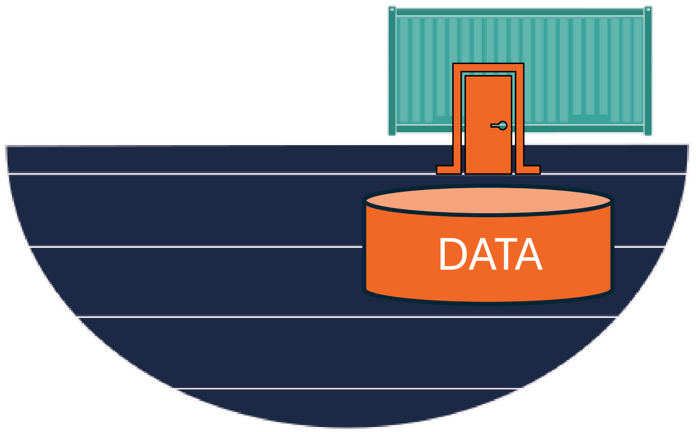
- Container is isolated from host
- Data in the container is NOT kept
- Solution:
  - Biding volume

    -v /path/in/host:/path/in/container

  - Naming volume

    -v volume_name:/path/in/container

```
docker run --detach \
-v MyVolume:/path/in/container/dataset \
--name <container_name> <container:version> <container_options>
```



ACTIVITY TIME:

- Activity 2.1
  - Run interactively and mount the **local data/** folder to the **container /data**
    - biocontainers/ fastqc:v0.11.9_cv7.
  - Remove the container after it has run

- Biding volume

-v /path/in/host:/path/in/container

- Activity 2.2
  - Do a quality control on the WT samples
    - Use the command

```
fastqc /data/WT_lib1_R1.fq.gz or fastqc /data/ecoli_1.fastq.gz.
```

- Why do we need to add **/data/** in the fastqc command?

ACTIVITY TIME: 3

- Who is the default user within the container?

- Run interactively and mount the local data/ directory to /scratch in the container
  - biocontainers/fastqc:v0.11.9_cv7

- In the container directory
  - Create a temporary file file1.txt in the scratch/

- Quit the interactive session.
  - On your host, check the file permissions.

- On the host
  - Create a temporary file file2.txt in the data/ directory.

- Run interactively and inspect the file permissions of this file
  - the fastqc container
- Check the file permissions of this file in the container (scratch/ directory).

- On the host, find out which UID and GID you have.
  - Tip: you can find your UID and GID with: id -u and id -g.

- Run a docker container by using the -u parameter
  - In the meantime creating a temporary file file3.txt with touch.
- Mount your current directory to /data
  - Within quay.io/biocontainers/fastqc:0.11.9--0.
  - Check the file permissions of this file in the container.

ACTIVITY TIME: 4

- Exercise 4.1
  - Execute the container: quay.io/biocontainers/fastqc:0.11.9_cv7
    - Use working directory option **-w** for a directory **scratch/**
    - Create a temporary file file4.txt with touch.
    - Mount your current directory to **scratch/** within the Docker container
    - Check the file location of this file on the host.

- Exercise 4.2
  - Execute the container: quay.io/biocontainers/fastqc:0.11.9_cv7
    - Use your user and group ID running
    - Do quality control of the file **WTXXX.fq.gz.**
    - mount your current directory to **the default working directory** within the Docker container
    - Verify that the HTML report is created with the correct file permissions.

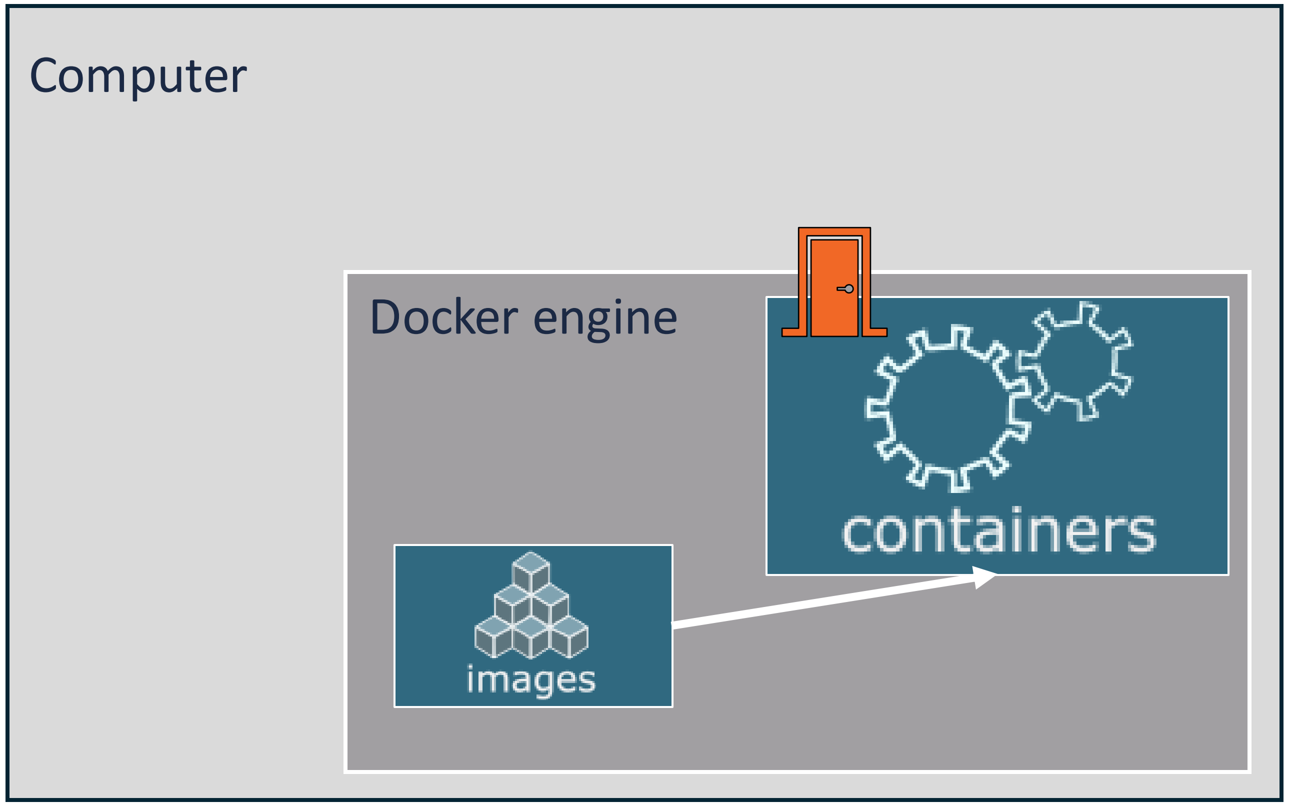
- **Extra:**
  - Can you analyze **all fastq** files using a glob-pattern (WT*.fq.gz)?
  - What do you need to change to make this work?

Ports

- Establish communication with webserver

```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```



Ports

- Stablish communication with webserver

```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```

Nginx (Engine-x) : creates a local webserver

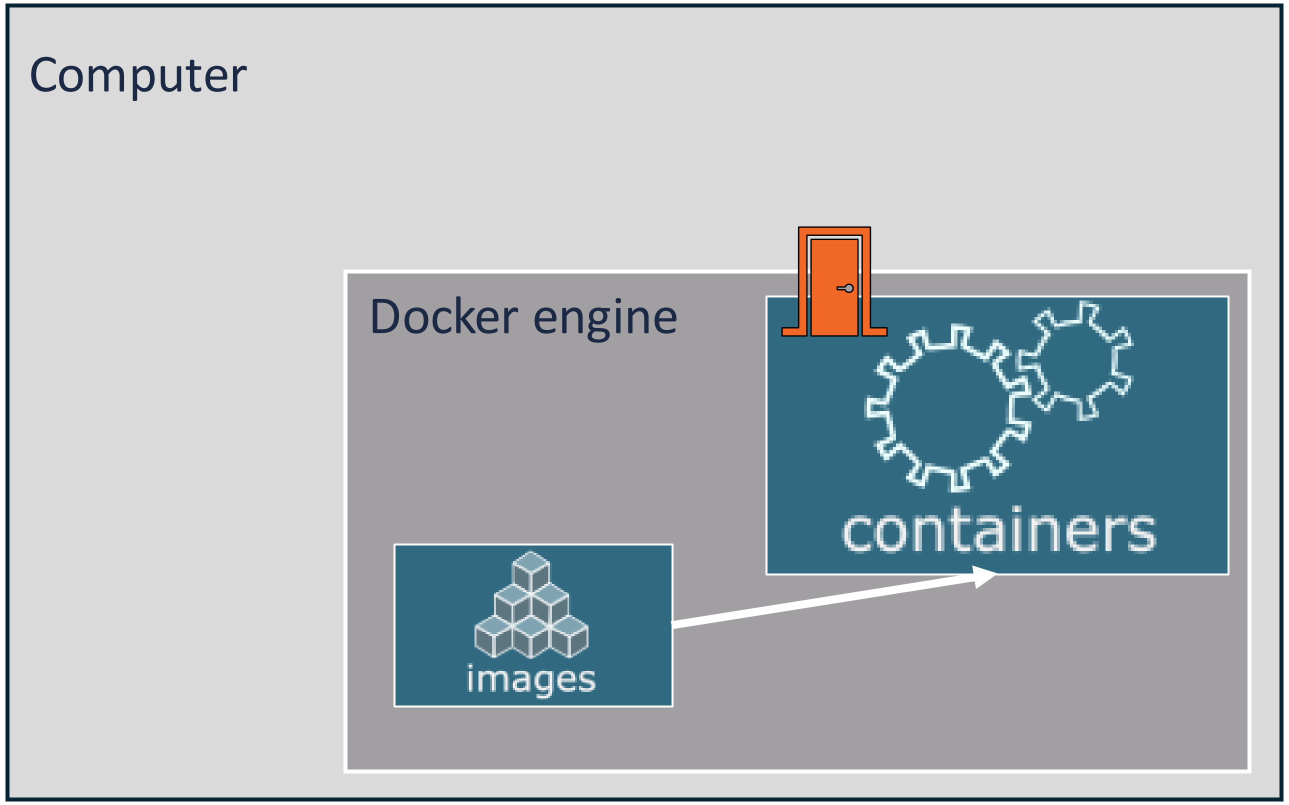
curl : Client URL

Enables communication between the host and the server

Practice time:

```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```



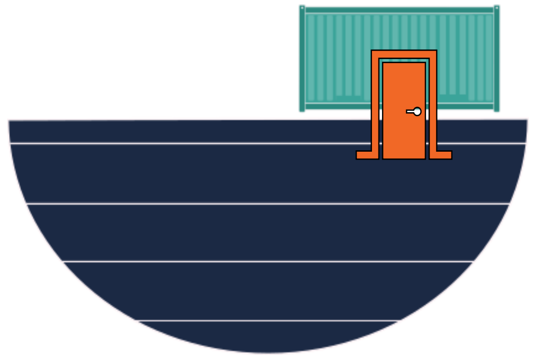
Ports

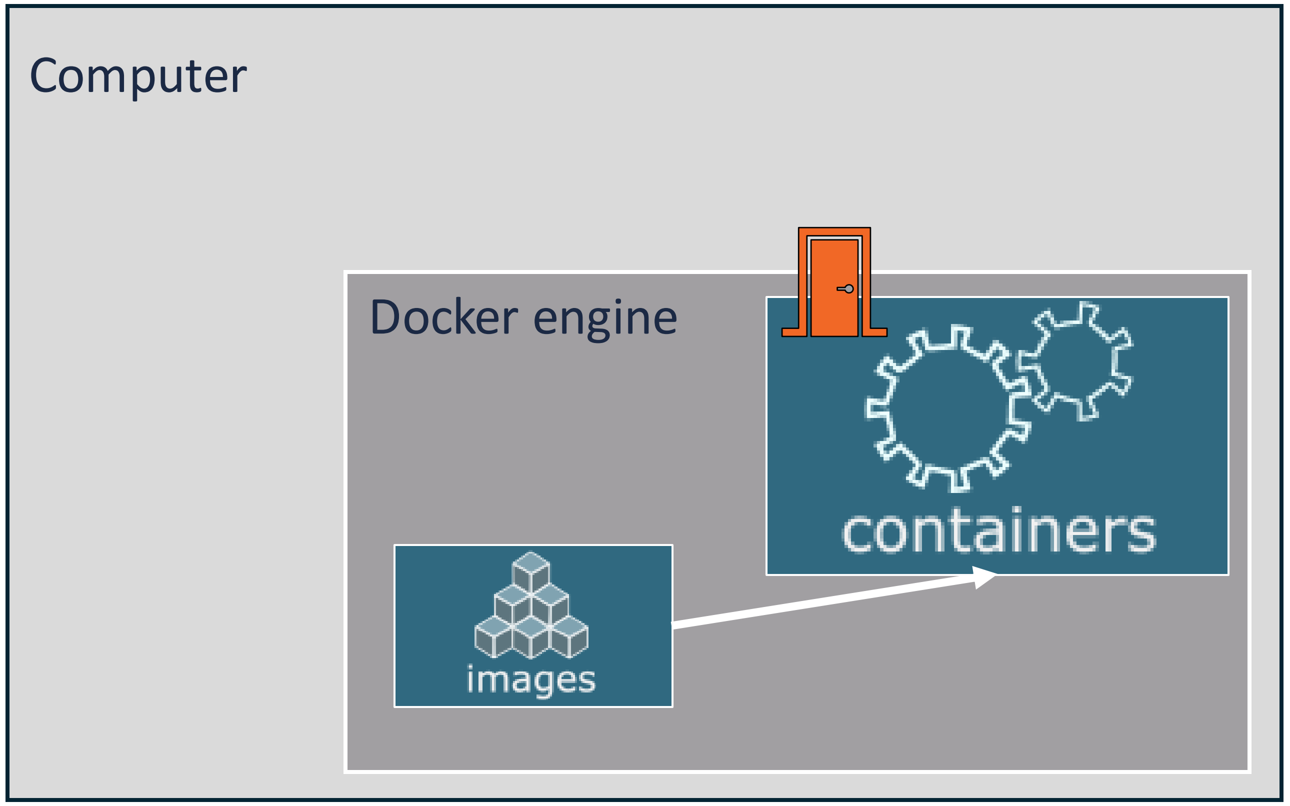
- Stablish communication with webserver

```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```

- Container X external environment



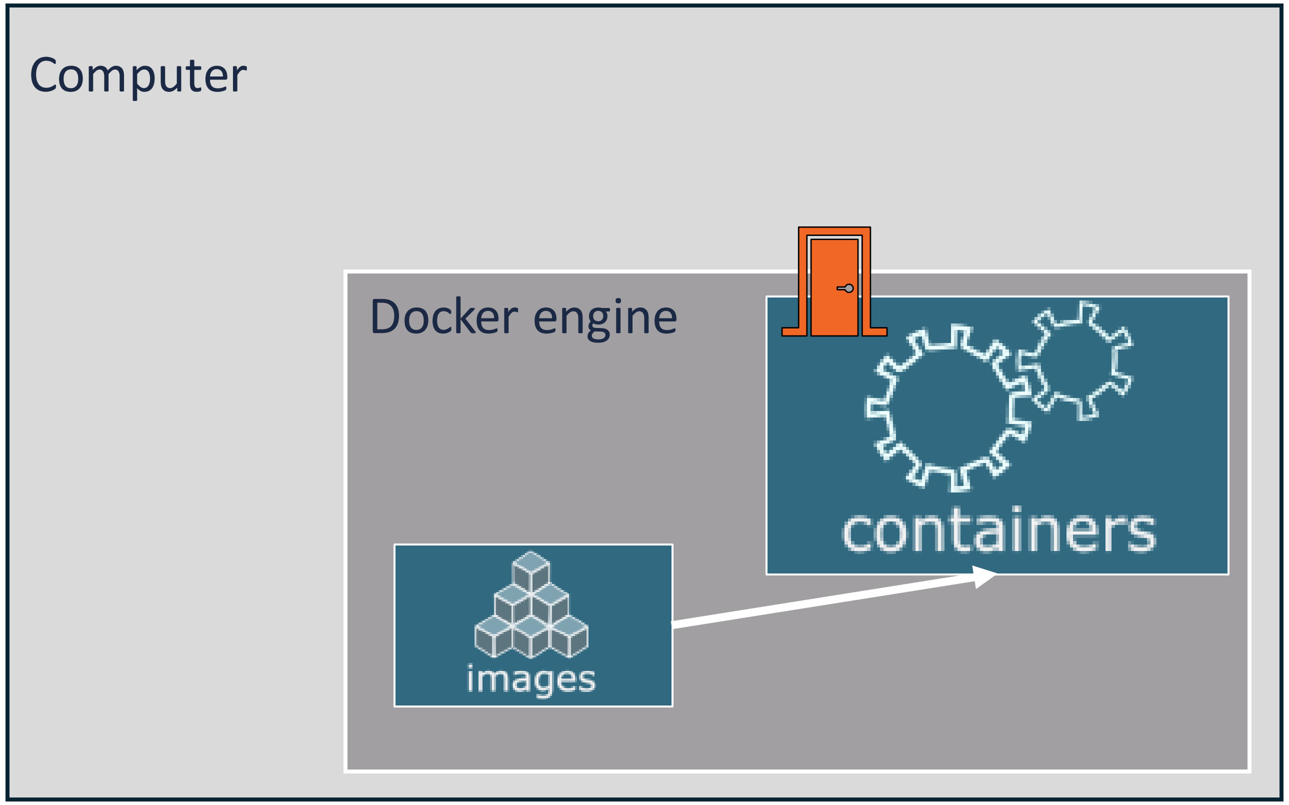


Practice time:

```
$ docker run --detach --name webserver nginx
```

```
$ docker exec webserver curl localhost:80
```

What is the difference between `run` and `exec`?



Ports

- Stablish communication with webserver

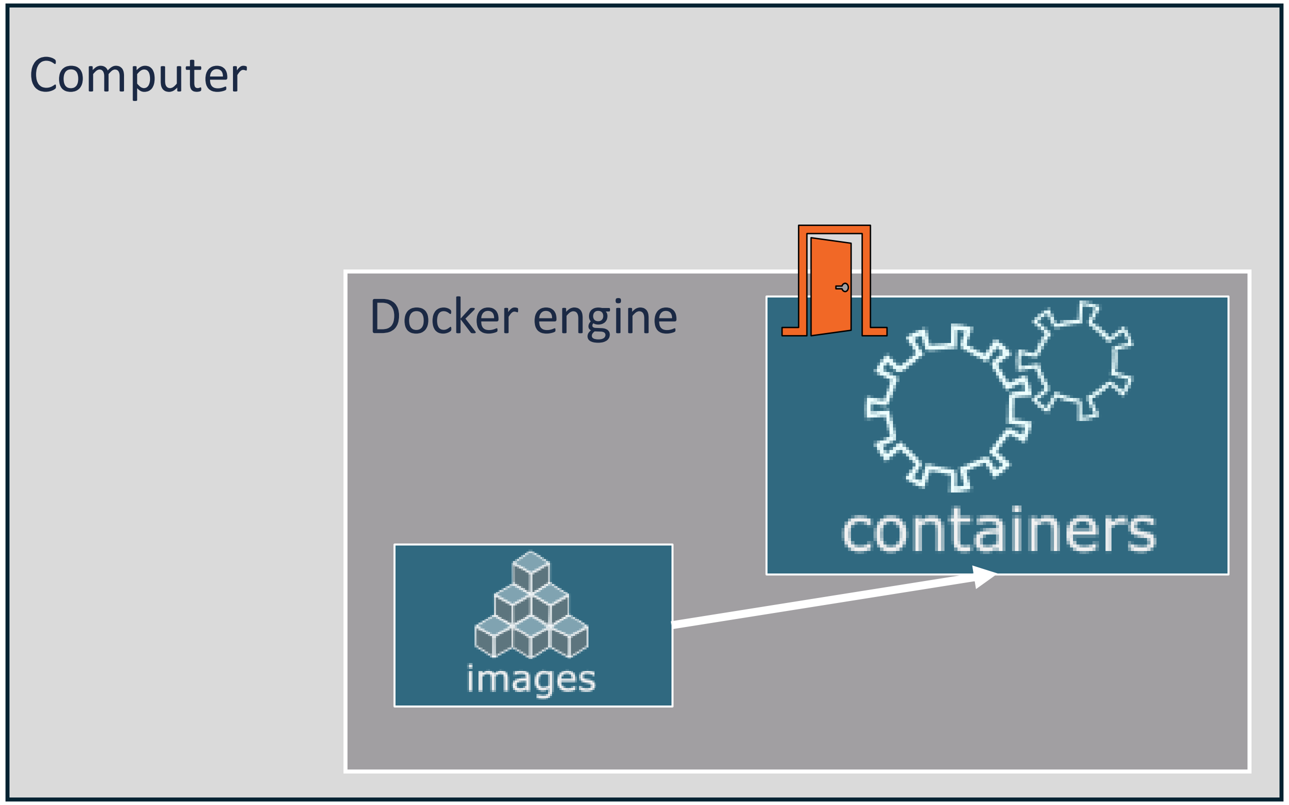
```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```

- Container X external environment

- exec : execute inside the container
    - Open the door for host communication

```
$ docker exec webserver curl localhost:80
```

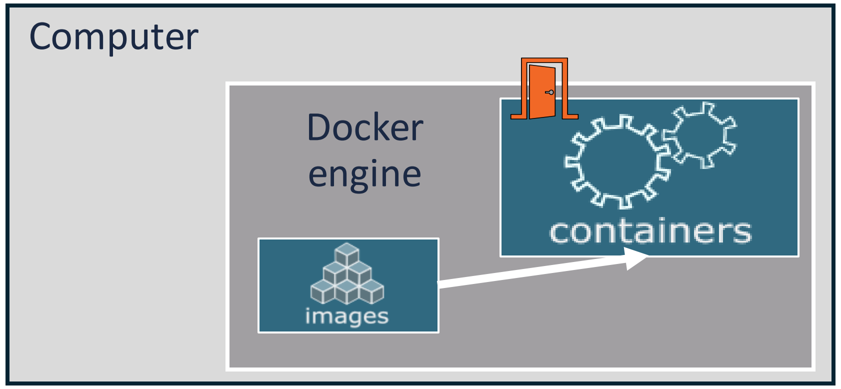


Ports

- To keep the door open

```
$ docker run --detach --name webserver --publish 80:80 nginx
```

```
$ curl localhost:80
```



Ports

- To keep the door open

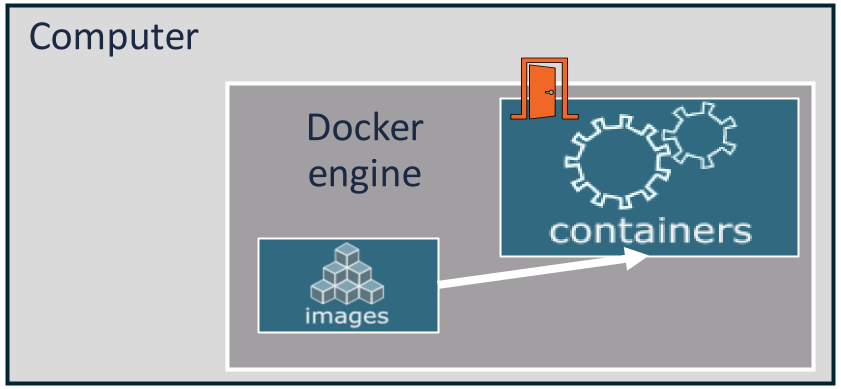
```
$ docker run --detach --name webserver --publish 80:80 nginx

$ curl localhost:80
```

```
$ docker run --detach --name webserver -p 8080:80 nginx

$ curl localhost: ????

$ docker exec webserver curl localhost: ???
```



FYI

--publish

=

-p

Practice time:

- What happens? Why?

```
$ docker run --detach --name webserver --publish 80:80 nginx

$ curl localhost:80
```

- What should you use? Why ?

```
$ docker run --detach --name webserver -p 8080:80 nginx

$ curl localhost: ????

$ docker exec webserver curl localhost: ???
```

Remember to remove these containers

docker rm -f <name>

Inspect

- Check a recipe
  - How others do
  - Potential security issues

```
$ docker inspect <image_name\image_ID>
```

Practice time:

- Find trimmomatic in docker hub
  - dceoy/trimmomatic
- Pull and inspect

```
FROM ubuntu:latest

ENV DEBIAN_FRONTEND noninteractive

ADD https://github.com/timflutre/trimmomatic/archive/master.tar.gz /tmp/trimmomatic.tar.gz

RUN set -e \
      && ln -sf bash /bin/sh

RUN set -e \
      && apt-get -y update \
      && apt-get -y dist-upgrade \
      && apt-get -y install --no-install-recommends --no-install-suggests \
        default-jdk make \
      && apt-get -y autoremove \
      && apt-get clean \
      && rm -rf /var/lib/apt/lists/*

RUN set -e \
      && tar xvf /tmp/trimmomatic.tar.gz -C /opt --remove-files \
      && mv /opt/trimmomatic-* /opt/trimmomatic \
      && cd /opt/trimmomatic \
      && make

RUN set -e \
      && mkdir /opt/trimmomatic/bin \
      && echo '#!/usr/bin/env bash' > /opt/trimmomatic/bin/trimmomatic \
      && echo 'java -jar /opt/trimmomatic/classes/trimmomatic.jar ${@}' \
        >> /opt/trimmomatic/bin/trimmomatic \
      && chmod +x /opt/trimmomatic/bin/trimmomatic

ENV PATH /opt/trimmomatic/bin:${PATH}

ENTRYPOINT ["/usr/bin/java", "-jar", "/opt/trimmomatic/classes/trimmomatic.jar"]
```

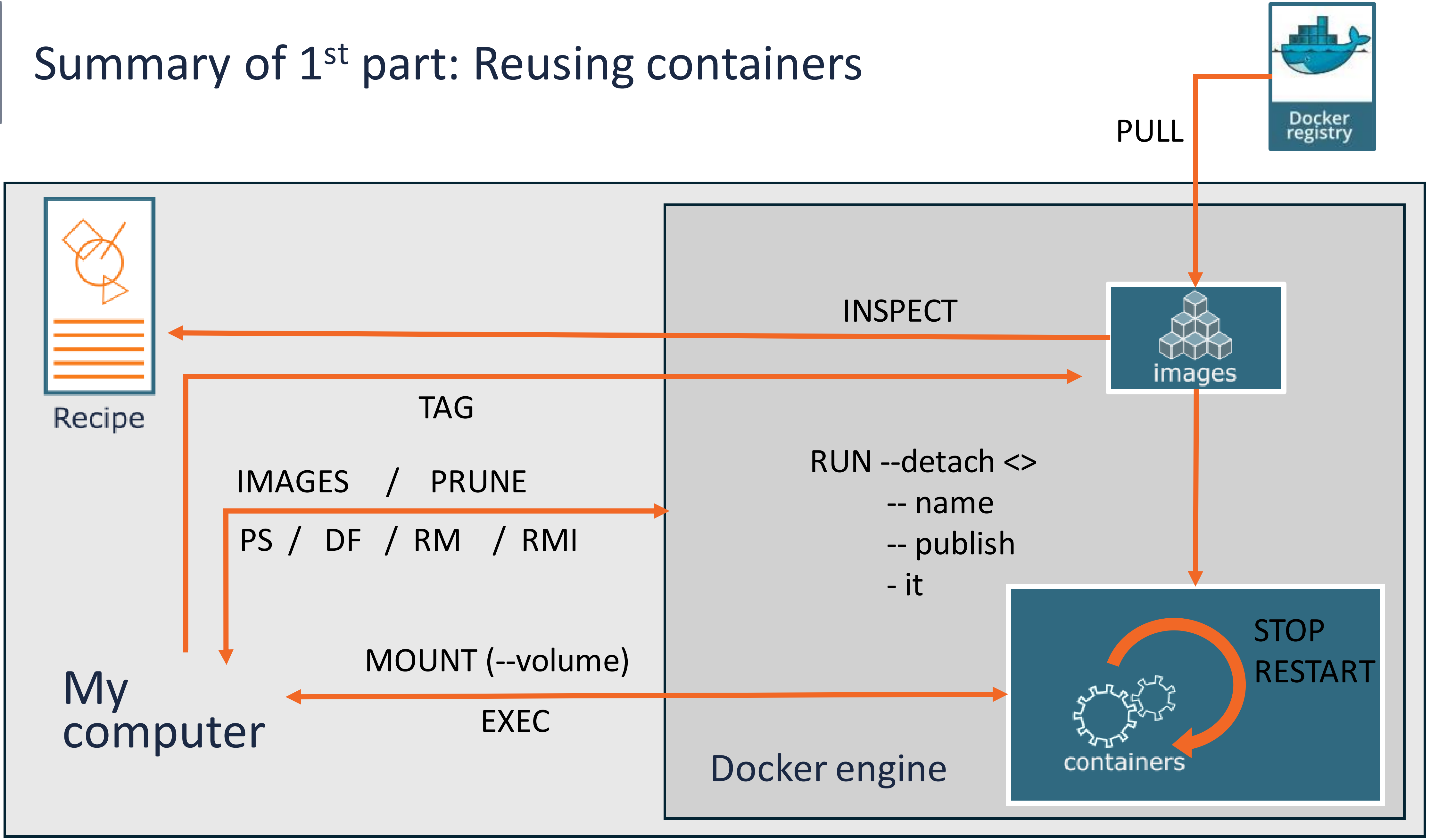
ACTIVITY TIME: 4.3 + challange

- Inspect the image biocontainers/fastqc:0.11.9_cv7
- Extract the working directory (WorkingDir) using grep.

HINT:

```
cmd | grep “keyword”
```

Summary of 1st part: Reusing containers

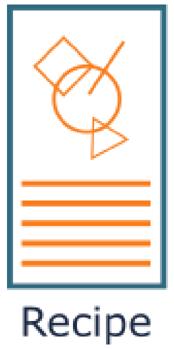


Building your own docker image

Barcelona-2023_byBpiereck

Recipes

- The default recipe is called Dockerfile



```
FROM ubuntu:18.04

RUN apt update && apt -y upgrade
RUN apt install -y wget
```

Practice time: Building images

- Create a Dockerfile with the content below in a folder of your preference and save it.

```
FROM ubuntu:18.04

RUN apt update && apt -y upgrade
RUN apt install -y wget
```

- How many layers should be created?

Practice time: Building images

- Let’s test it and build the image with

```
docker build .
```

- How many layers should be created?

```
docker history <id>
```

Practice time: Building images

- Create a Dockerfile with the content below in a folder of your preference and save it.

```
FROM ubuntu:18.04

LABEL org.opencontainers.image.authors=”training@vib.be"


WORKDIR ~

RUN apt update && apt -y upgrade
RUN apt install -y wget

ENTRYPOINT ["/usr/bin/wget"]
CMD ["https://cdn-images-1.medium.com/max/1600/1*_NQN6_YnxS29m8vFzWYlEg.png"]
```

Build the image with and without caching.

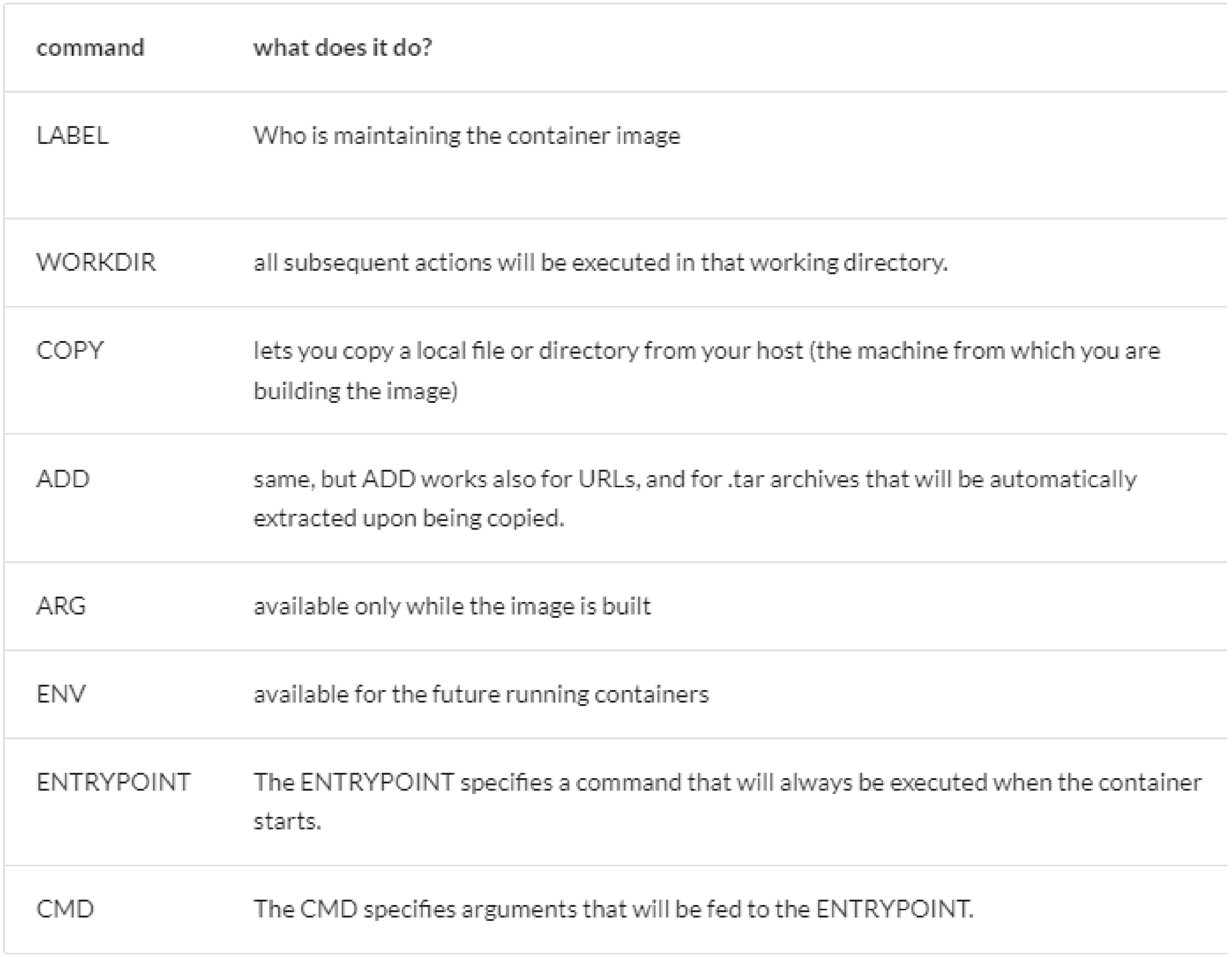
Recipes

Recipe

images

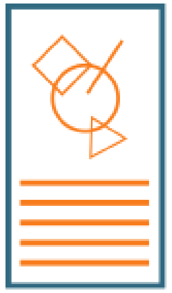
More advanced image building

- Different ways to build images.
- Know your base system and their packages. Popular ones:
  - Debian
  - CentOS
  - Alpine
  - Conda. Anaconda, Conda-forge, Bioconda, etc.



command	what does it do?
LABEL	Who is maintaining the container image
WORKDIR	all subsequent actions will be executed in that working directory.
COPY	lets you copy a local file or directory from your host (the machine from which you are building the image)
ADD	same, but ADD works also for URLs, and for .tar archives that will be automatically extracted upon being copied.
ARG	available only while the image is built
ENV	available for the future running containers
ENTRYPOINT	The ENTRYPOINT specifies a command that will always be executed when the container starts.
CMD	The CMD specifies arguments that will be fed to the ENTRYPOINT.

Recipes



One tool, one image or some tools, one image

- Different ways to build images.
- start from packages e.g. pip/PyPI, CPAN, or CRAN
- use versions for tools and images
- reduce size as much as possible
- keep data outside the image/container
- check the license
- make your container discoverable e.g. biocontainers, quay.io, docker hub

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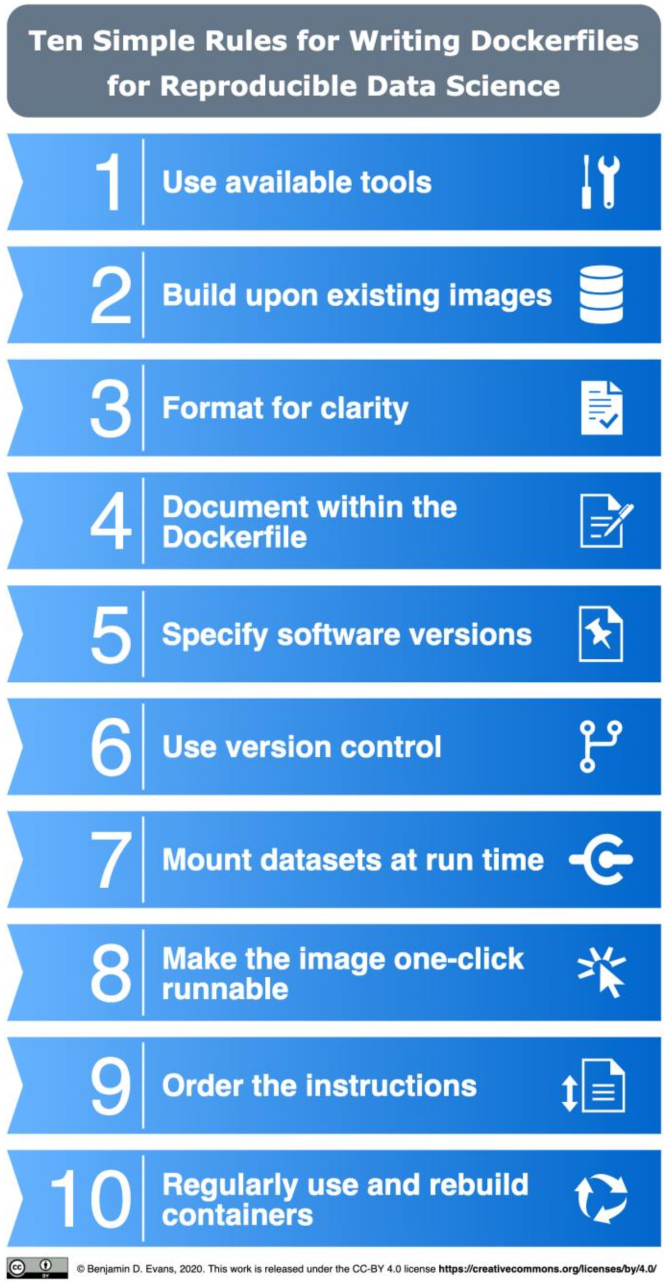
•https://doi.org/10.1371/journal.pcbi.1008316

Ten simple rules for writing Dockerfiles for reproducible data science

•Daniel Nüst,
•Vanessa Sochat,
•Ben Marwick,
•Stephen J. Eglen,
•Tim Head,
•Tony Hirst,
•Benjamin D. Evans



Ten Simple Rules for Writing Dockerfiles for Reproducible Data Science

1. Use available tools
2. Build upon existing images
3. Format for clarity
4. Document within the Dockerfile
5. Specify software versions
6. Use version control
7. Mount datasets at run time
8. Make the image one-click runnable
9. Order the instructions
10. Regularly use and rebuild containers

Recipe

images

https://docs.docker.com/engine/userguide/eng-image/dockerfile_best-practices/

ACTIVITY TIME: 5

- Exercise 5.1
  - Imagine the following situation. To make a simple data analysis project as reproducible as possible, we propose to create a container environment using Docker which contains the necessary tools and scripts. We have two use cases:
    - a) we would like to run the Python scripts on the command line
    - b) we think that a Jupyterlab is useful environment to play around with the data analysis.
      - Look for the Dockerfile.play in the folder docker

- Exercise 5.2
  - Once you have built an image based on the corrected Dockerfile, run the script data/codereppy_min_batch.py with the Python version installed in the image.
    - Reach out to your neighbour(s) in case you need help.

Recipes

One tool, one image or some tools, one image

- Different ways to build images.
- start from packages e.g. pip/PyPI, CPAN, or CRAN
- use versions for tools and images
- reduce size as much as possible
- keep data outside the image/container
- check the license
- make your container discoverable e.g. biocontainers, quay.io, docker hub

Short intro to HPC

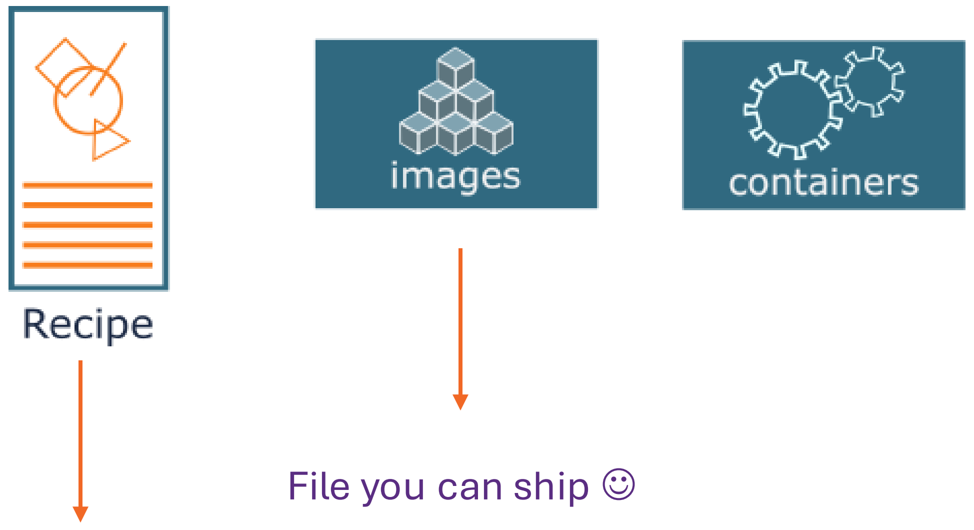
preparing for Apptainer

To be added

Introduction to Apptainer for reproducible analysis

How does it work?

- Important concepts
  - **Text file**: Your recipe
  - **Apptainer image:** Static file
  - **Container:** Running image (functional)



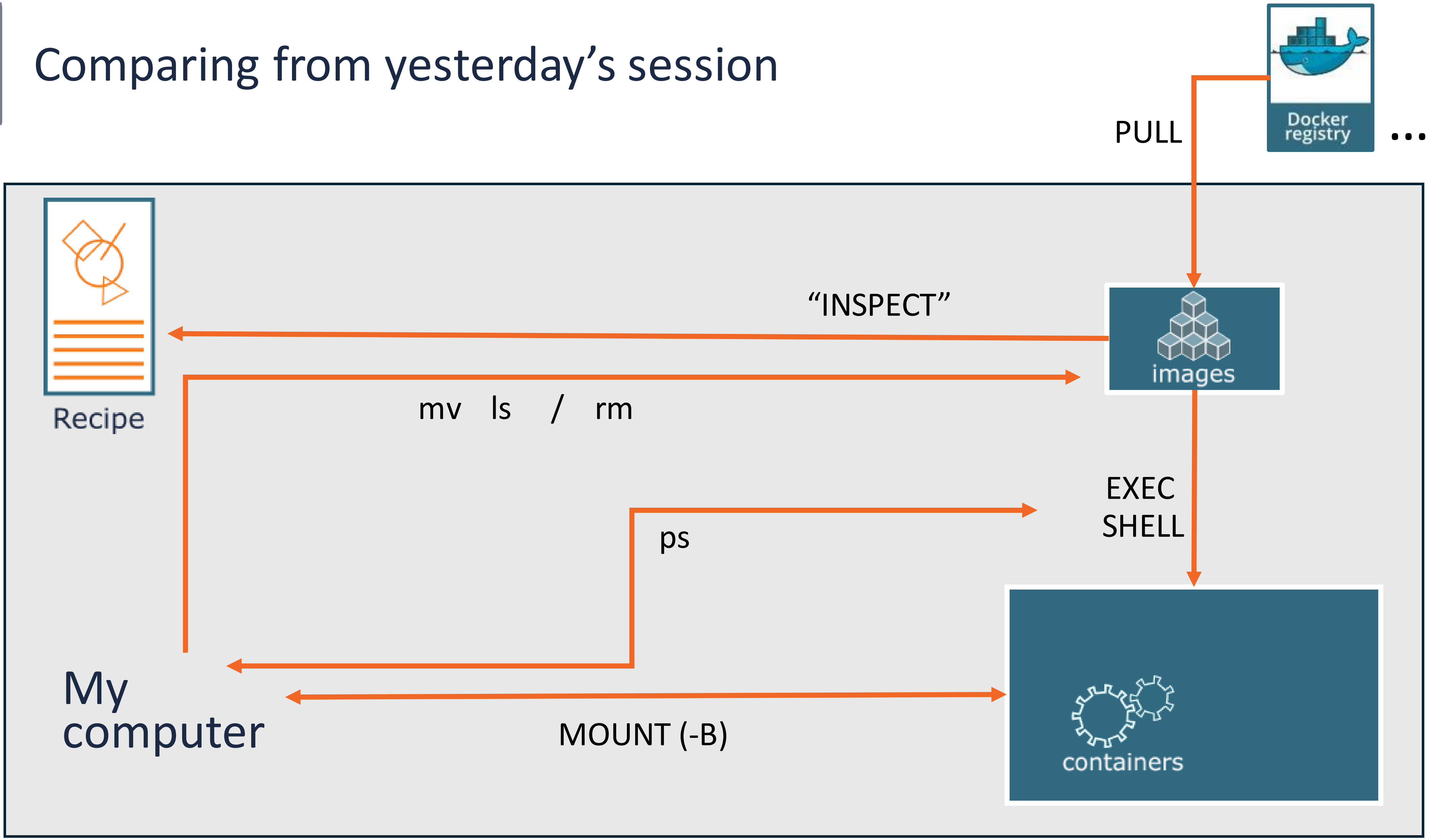
File you can ship ☺

your recipe to build

the Apptainer

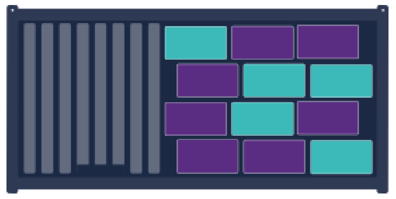
image

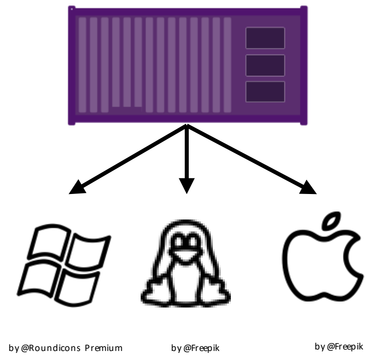
Comparing from yesterday's session



Docker vs Apptainer

- **Strengths**
- No dependency of a daemon
- Can be run as a simple user
  - Avoid permission headaches and hacks
- Image/container is a file (or directory)
- More easily portable
- Two type of images
  - Read-only (production)
  - Writable (development, via sandbox)
- **Weaknesses**
- At the time of writing only good support in Linux
- For some features you need root account (or sudo)





How does it work?

- By default, Apptainer uses $HOME/.apptainer/cache as the location for the cache.

  This will not work on the VSC.

  You can change the location of the cache by setting the $APPTAINER_CACHEDIR environment variable to the cache location you want to use.

- Please set the variable $APPTAINER_CACHEDIR to $VSC_SCRATCH.

Practice time: 1

- **Exercise 1**
- In the hello world container, try editing (for example using the editor vi which should be available in the container) the /rawr.sh file. What do you notice?

- **Exercise 2:**
- In your home directory within the container shell, try and create a simple text file. Is it possible to do this? If so, why? If not, why not?! If you can successfully create a file, what happens to it when you exit the shell and the container shuts down?

Practice time: Downloading images

```
$ mkdir $VSC_DATA/apptainer-course
$ cd $VSC_DATA/apptainer-course
$ apptainer pull hello-world.sif shub://vsoch/hello-world
```

```
$ apptainer pull --name fastqc-0.11.9--0.sif https://depot.galaxyproject.org/singularity/fastqc:0.11.9--0
$ file fastqc-0.11.9--0.cif
```

Practice time: Binding folders

```
singularity shell -B /data/leuven/315/vsc315XX hello-world.sif

Singularity> ls /data/leuven/315/vsc315XX
```

```
$ singularity shell -B /data/leuven/315/vsc315XX :/shared-data hello-world.sif

Singularity> ls /shared-data
```

Practice time: Downloading images or pulling or building images

- Pulling images may take a while, so we need to run this as a job.

- qsub pull-image.pbs

```
...
APPTAINER_CACHEDIR=$VSC_SCRATCH \
APPTAINER_TMPDIR=$VSC_SCRATCH \
apptainer build --fakeroot $VSC_SCRATCH/tensorflow-23.06-tf2-py3.sif \
docker://nvcr.io/nvidia/tensorflow:23.06-tf2-py3
...
```

Practice time: And now really building images

- Pulling images may take a while, so we need to run this as a job.

- qsub build-image.pbs

- …

```
APPTAINER_CACHEDIR=$VSC_SCRATCH \
APPTAINER_TMPDIR=$VSC_SCRATCH \
apptainer build --fakeroot $VSC_SCRATCH/test_image_ubuntu.sif \
$VSC_SCRATCH/test_image_ubuntu.def
```

…