Barcelona-2023_byBpiereck

Introduction to Docker for reproducible analysis

VIB technologies

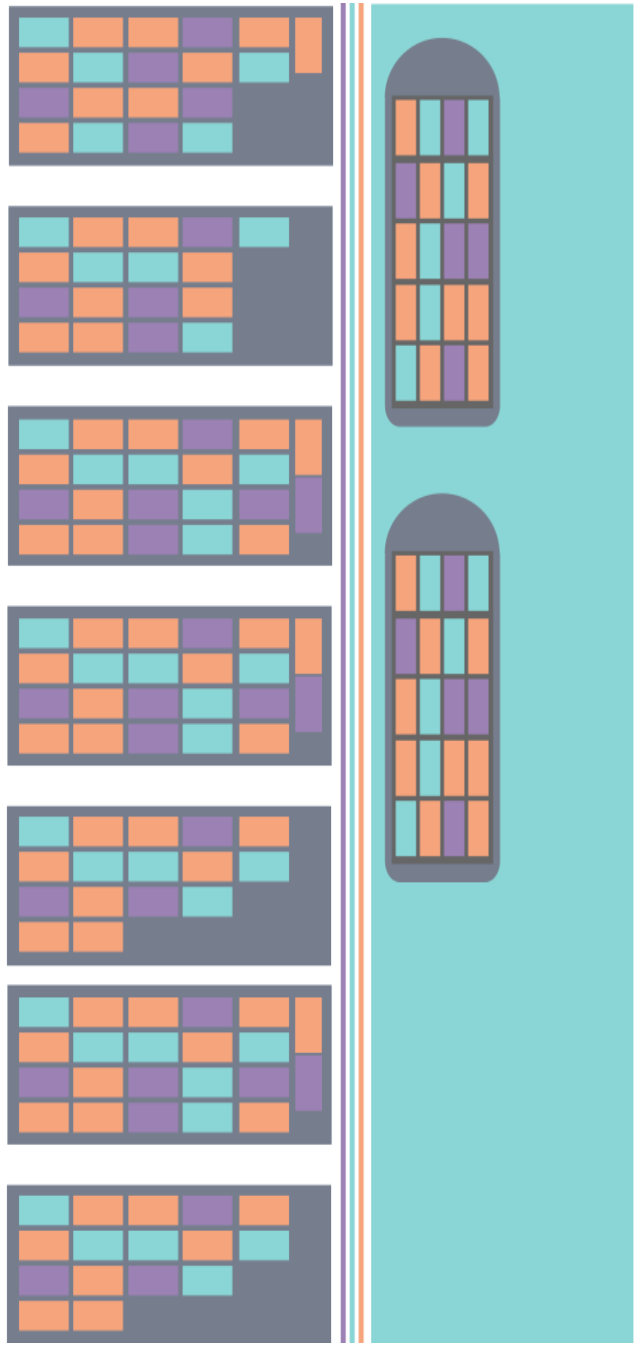
ELIXIR BELGIUM

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.



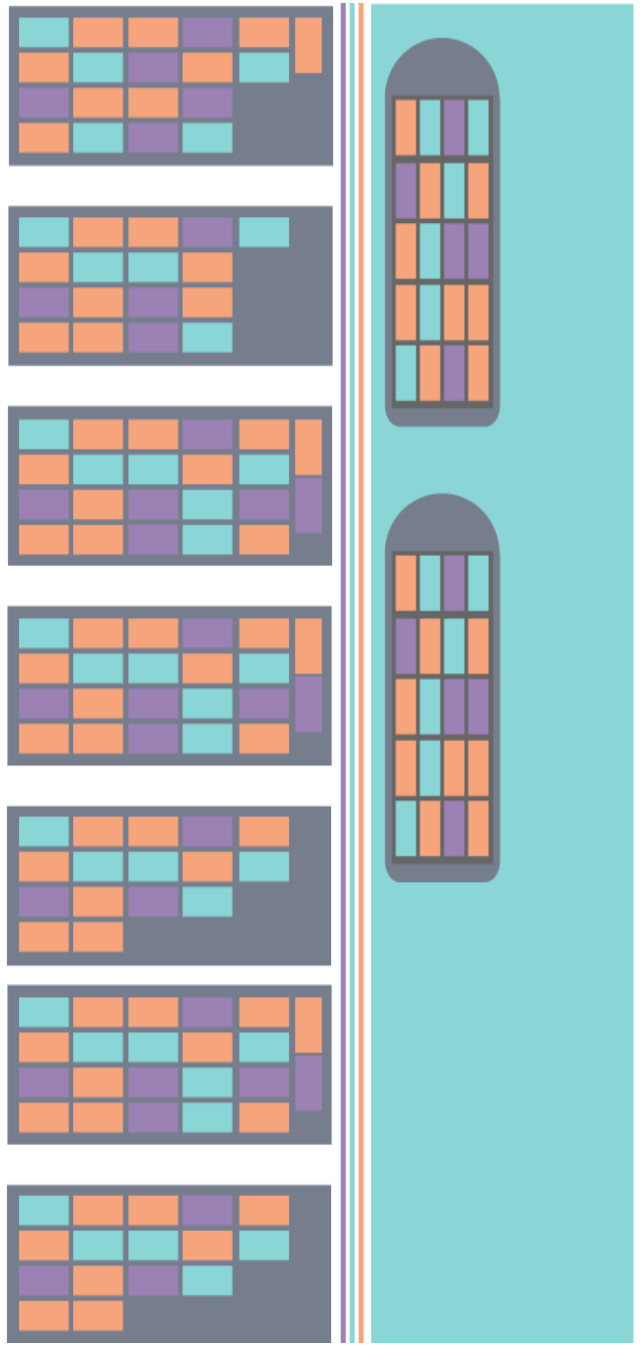
What is a DOCKER ?

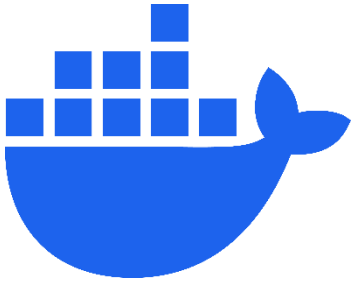
- Common definition: Person working in a port, responsible for **LOADING** and **UNLOADING** containers.

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.





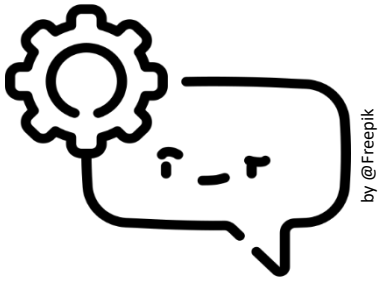
What is a container ?

> *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*

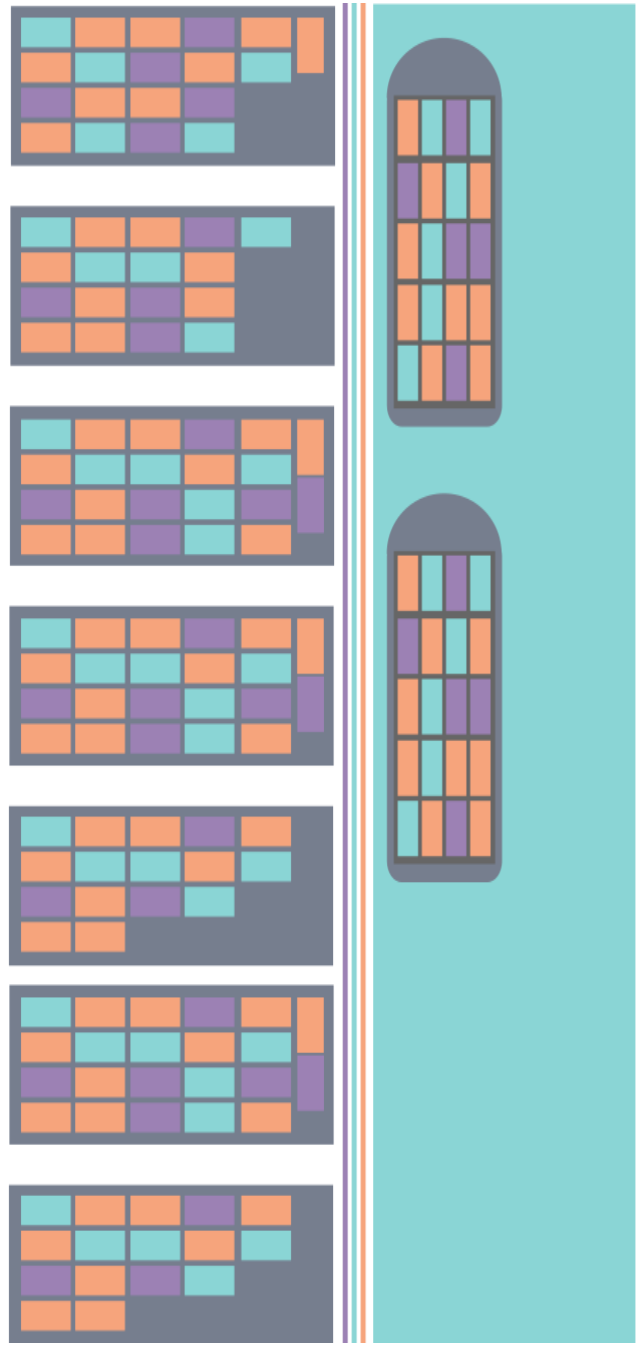
- https://www.docker.com/what-container -

p.s: Commercial use of Docker Desktop requires a paid subscription

“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

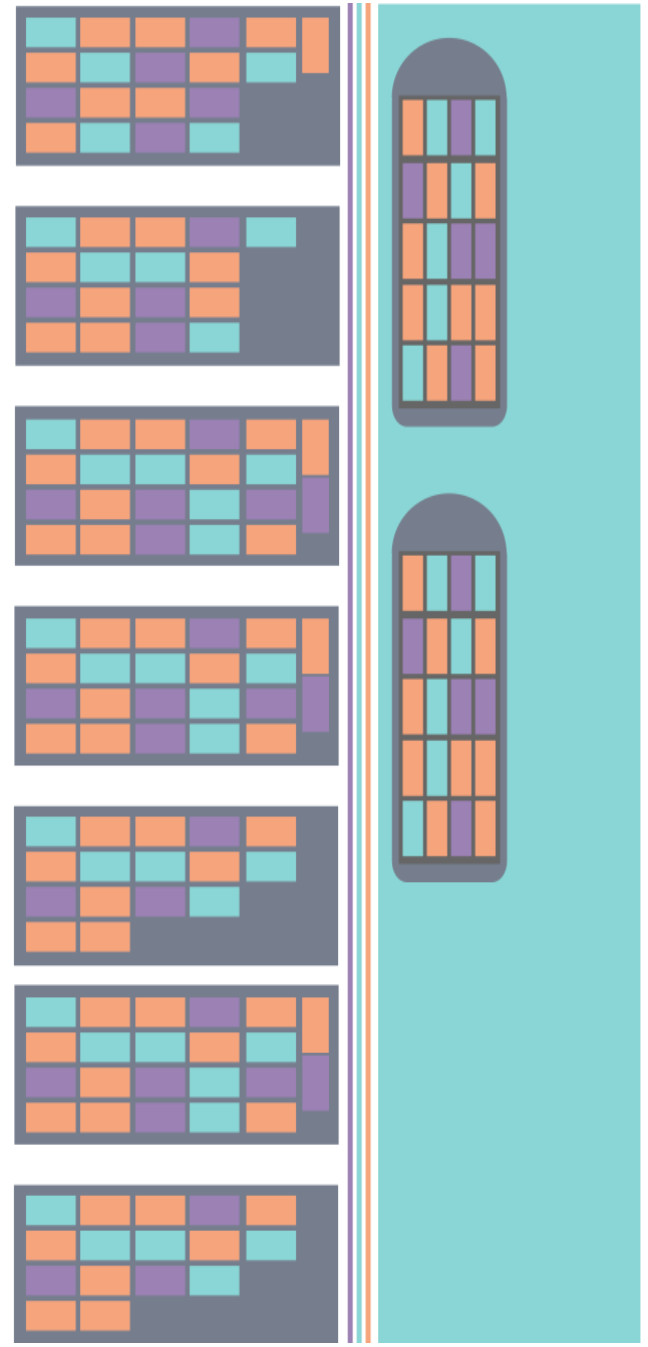
- Testing & continuous integration
  - Jenkins, Drone CI


by @Freepik

- Difficult to compile apps
  - PennCNV, hap.py

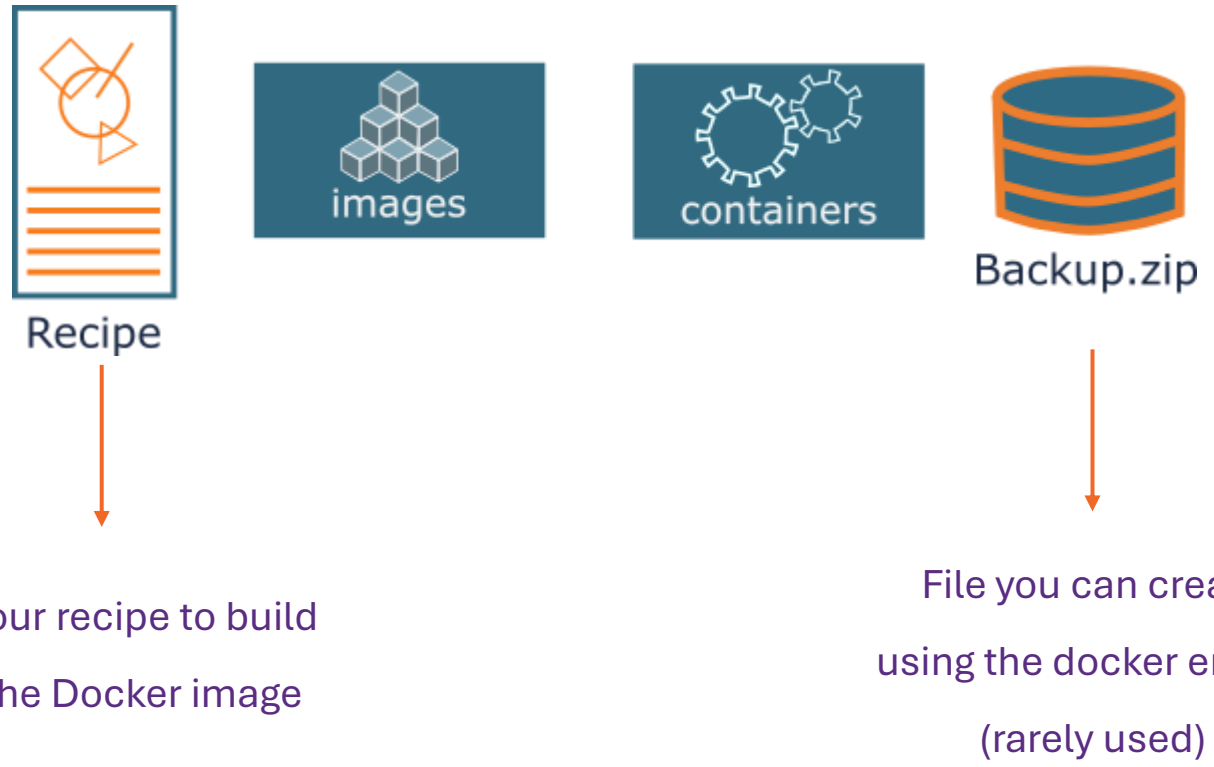

by @Creaticca Creative Agency

- 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’



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- Used as base
- Long-term storage

- Based on image
- Short lived

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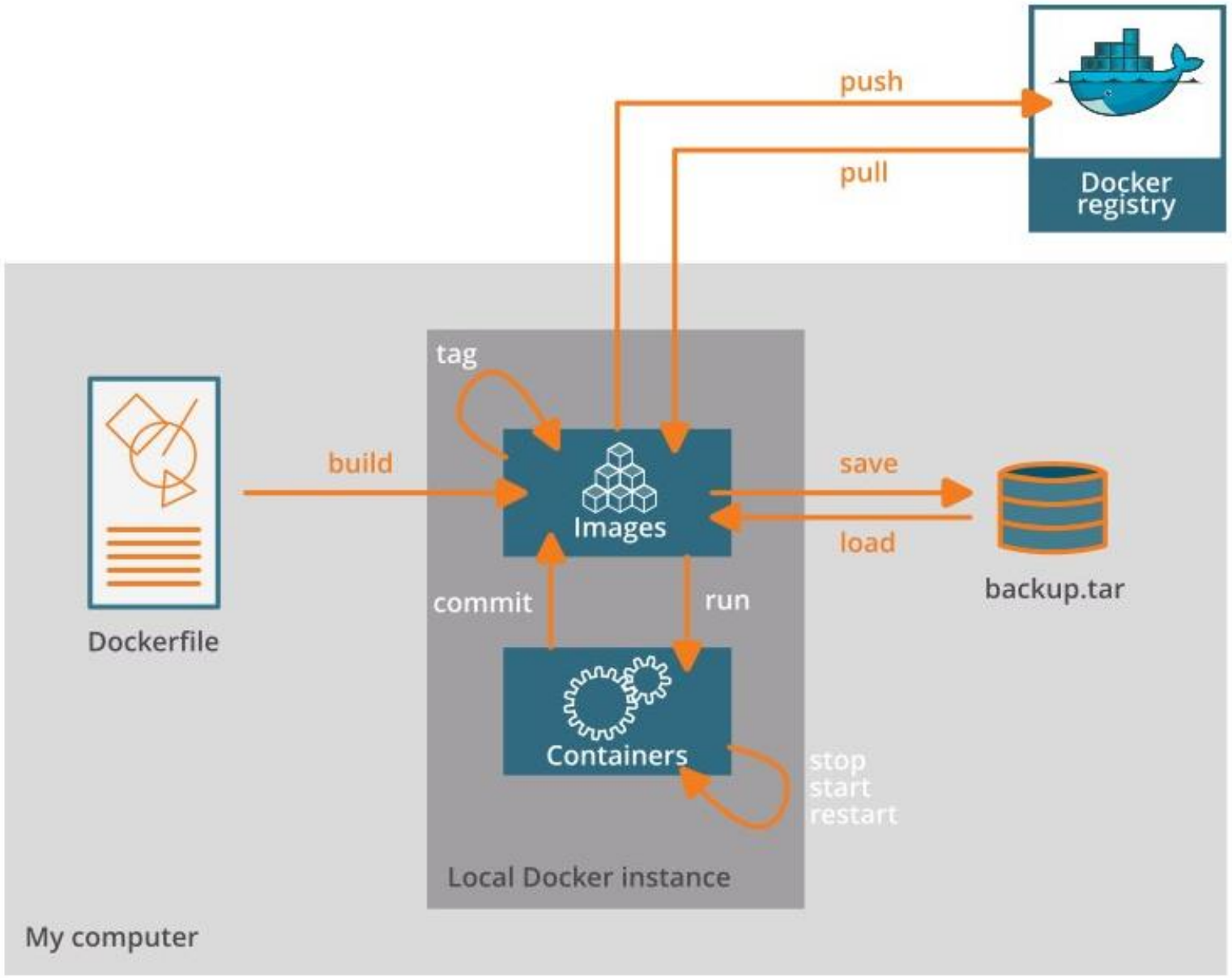

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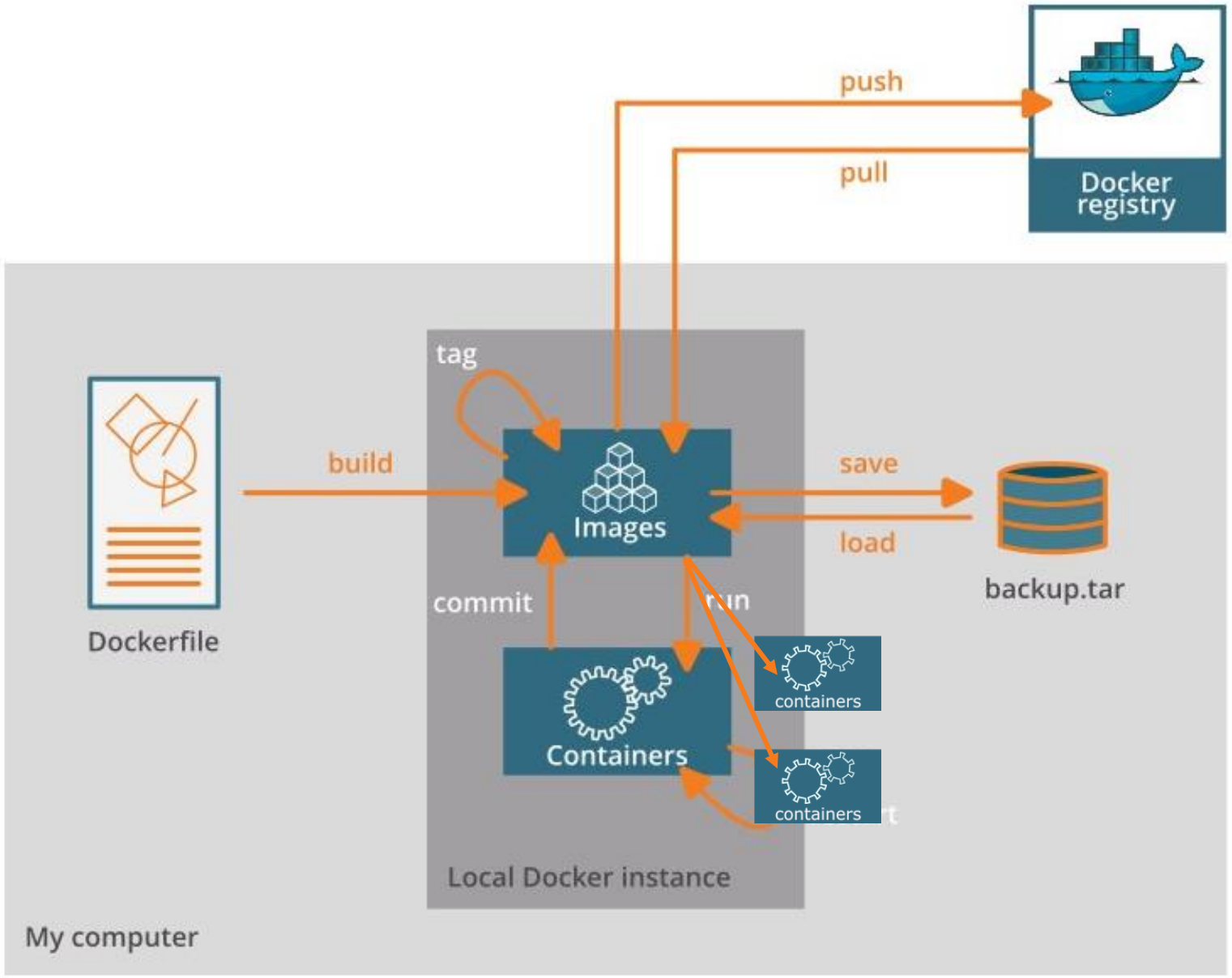

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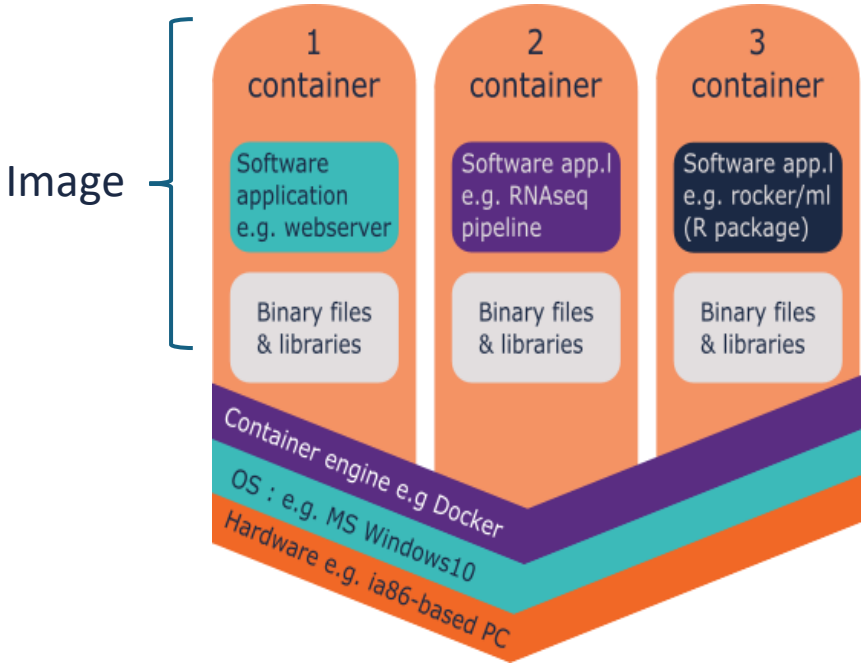
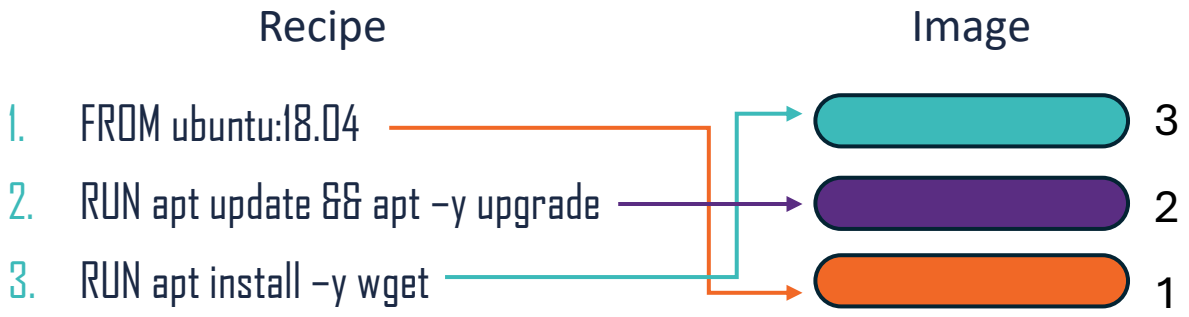
How is it organized?

- General components



- Docker images layers



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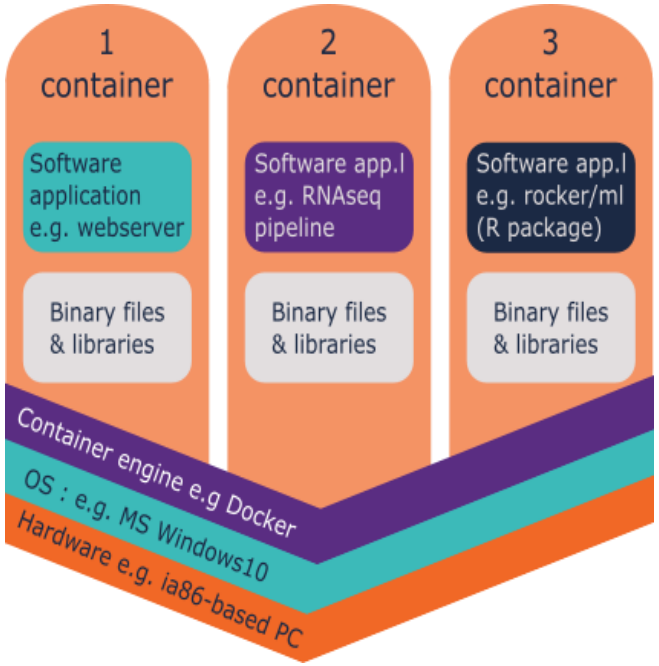

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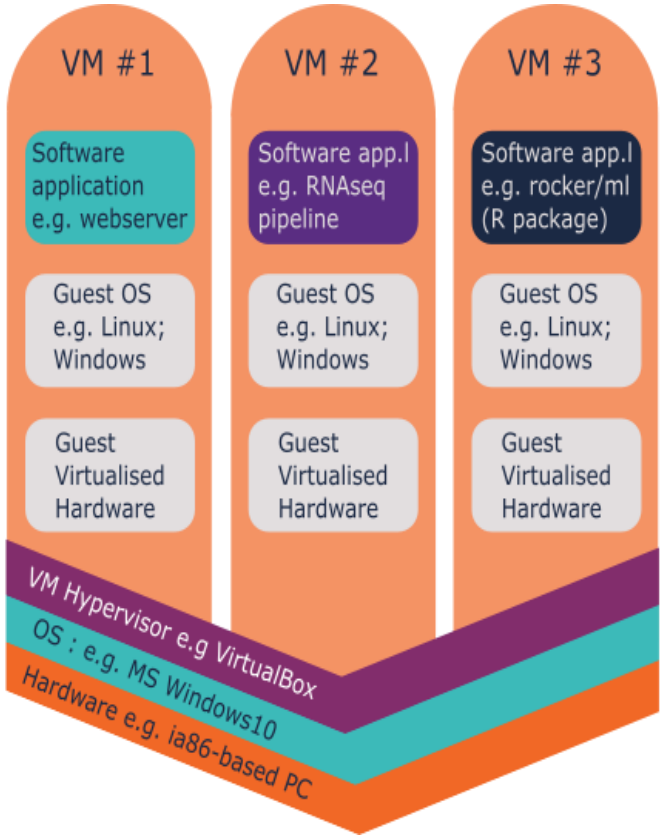
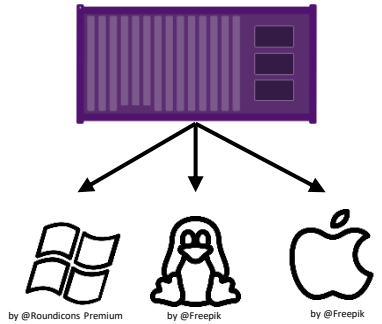


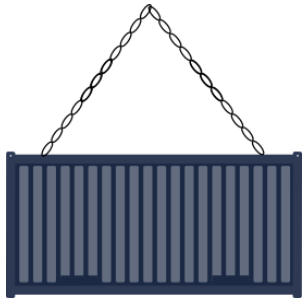
Advantages

- **Bundled Dependencies**
  - Contain all their dependencies = installing hurdles

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



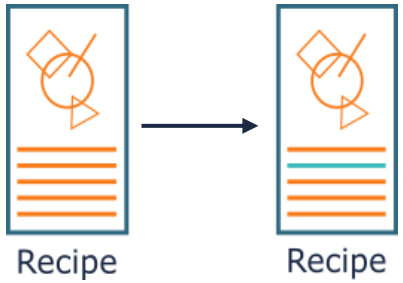
- **Easy Distribution**
  - Shared on Docker Hub or as ‘image.tar’ file



Advantages

- **Safety**
  - Can’t access files on the host machine

- **Ease-of-Use**
  - Can always be run using one single command

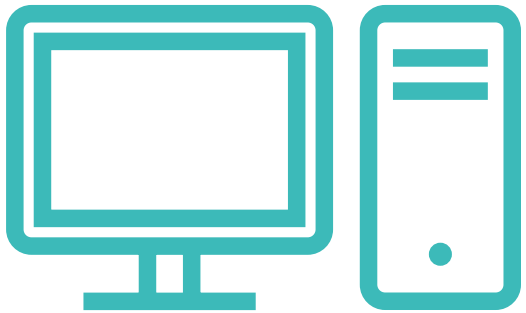


- **Easy Upgrades**
  - Easily swapped out for newer versions
  - All persistent data can be retained in a data volume

Other container software

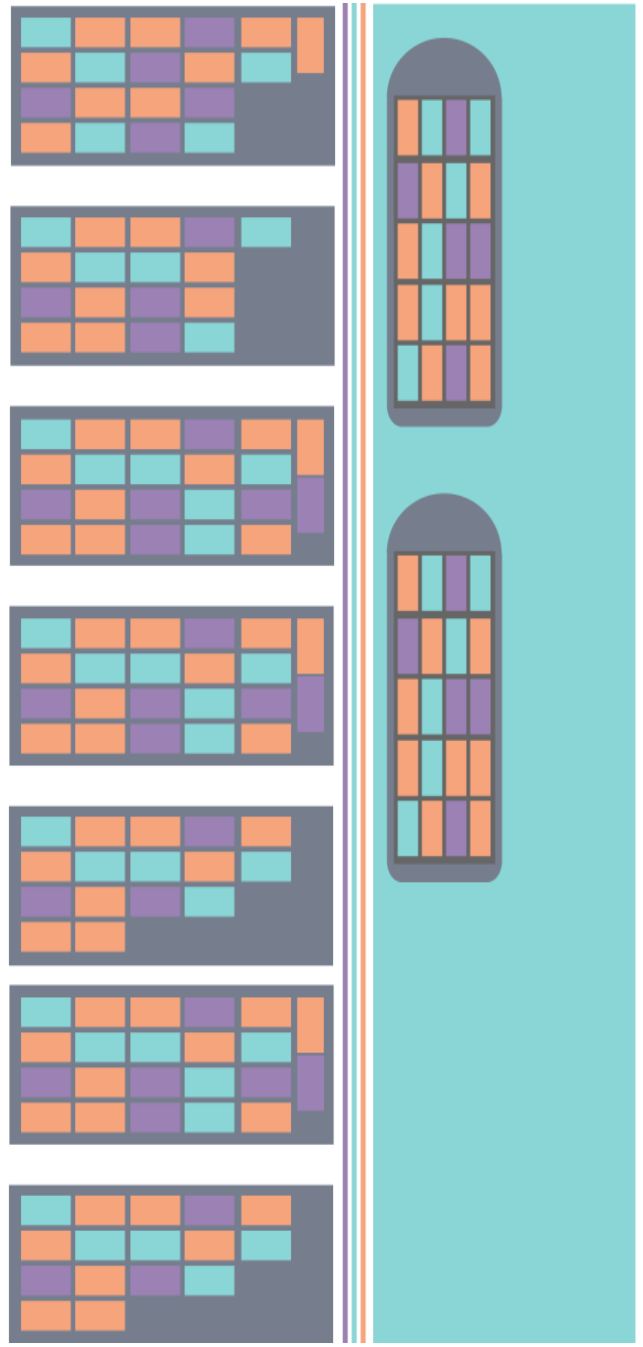
Using and Reusing available docker images

Where can we storage and find Docker images?



Local storage

Registry



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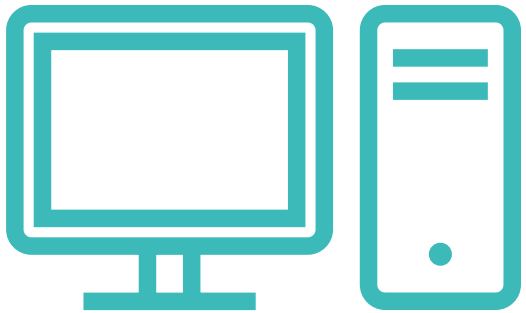

Local storage

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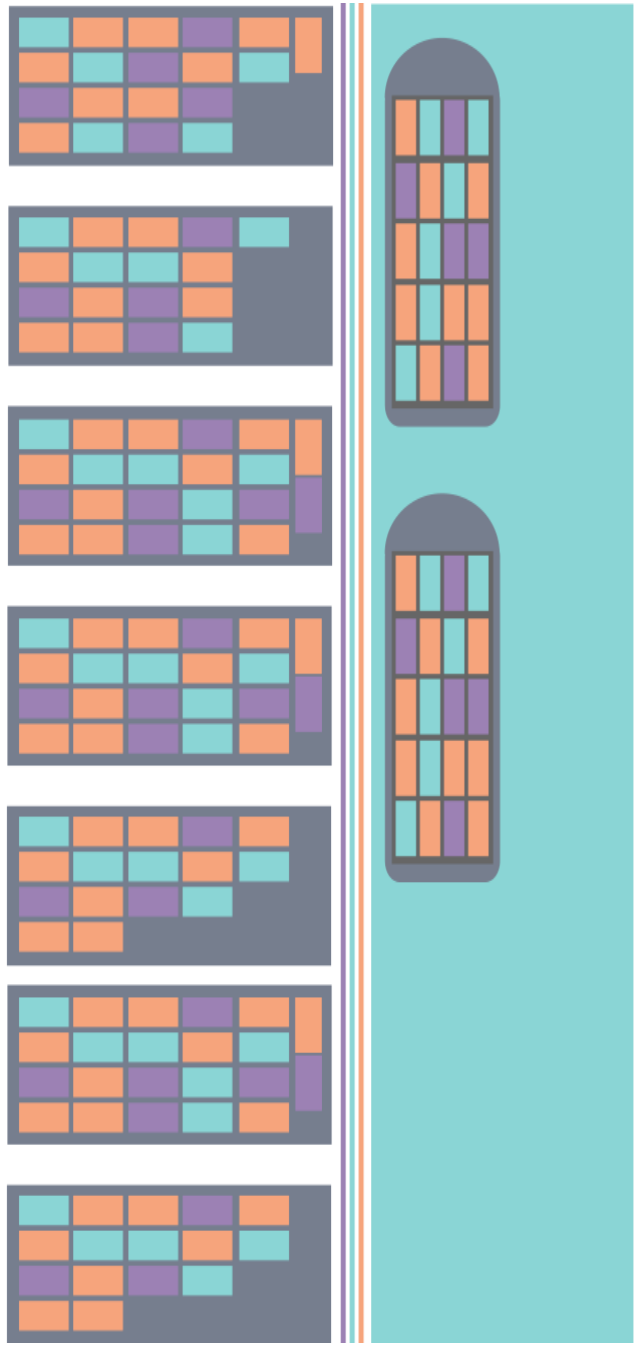
Preferable



Container Registries

- Main registry for DOCKER containers

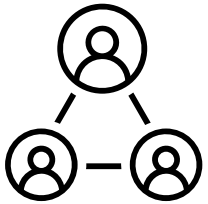
- Alternative registries

Container Registries

BioContainers

- Main registry for DOCKER containers

docker hub



docker hub

QUAY

- Alternative registries

Azure Container Registry

QUAY

HARBOR

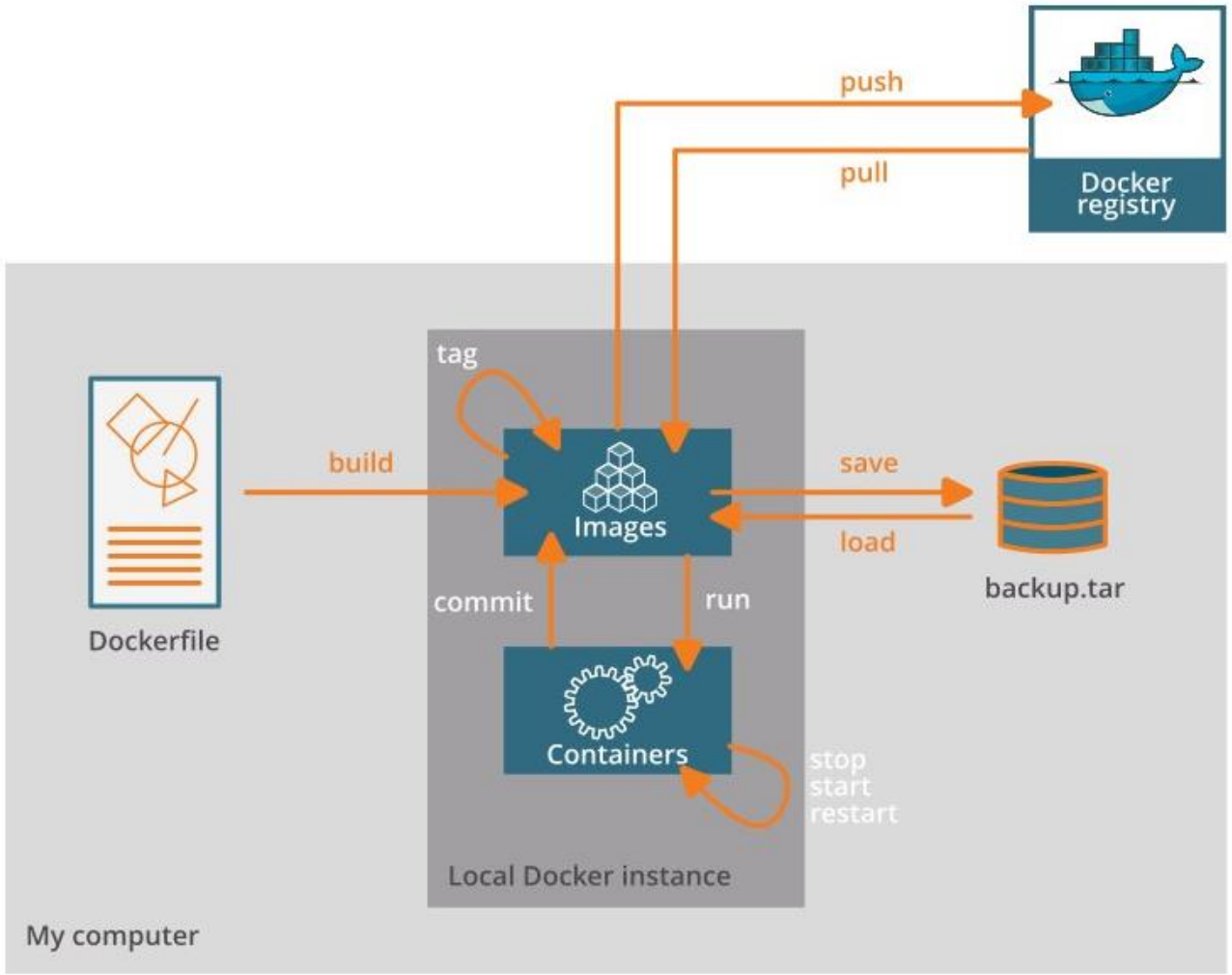
Google Container Registry

Gitlab Container Registry

JFrog

Amazon ECR

How do we get a container image?



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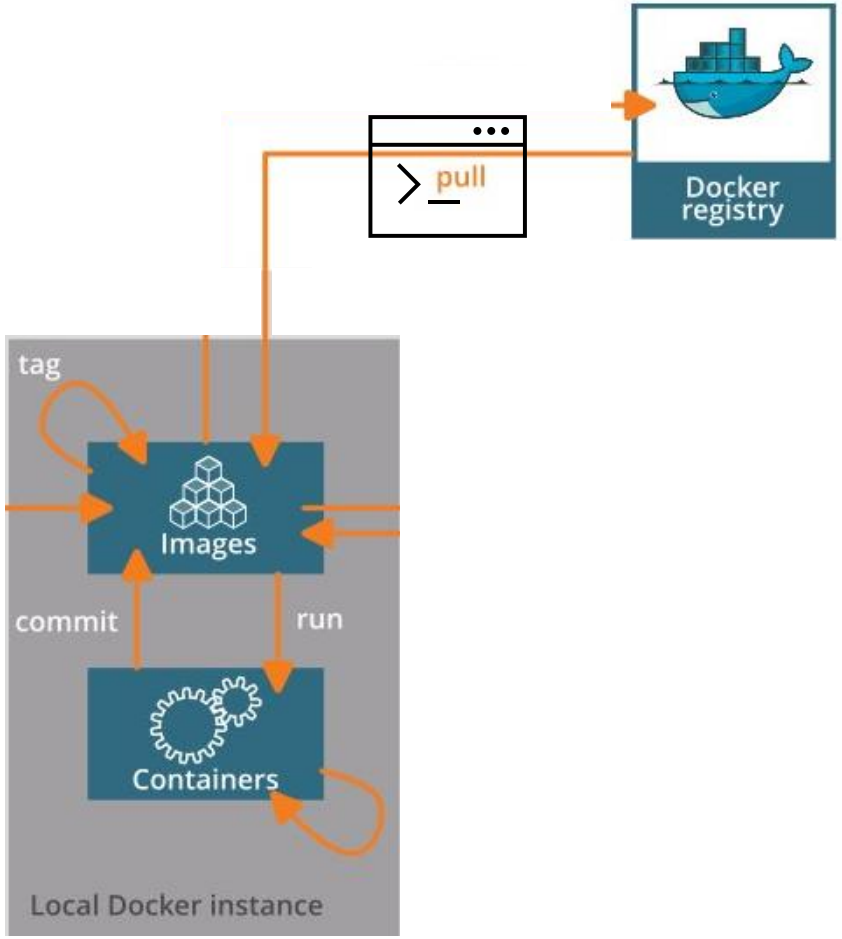
How do we get a container image?

- 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
```



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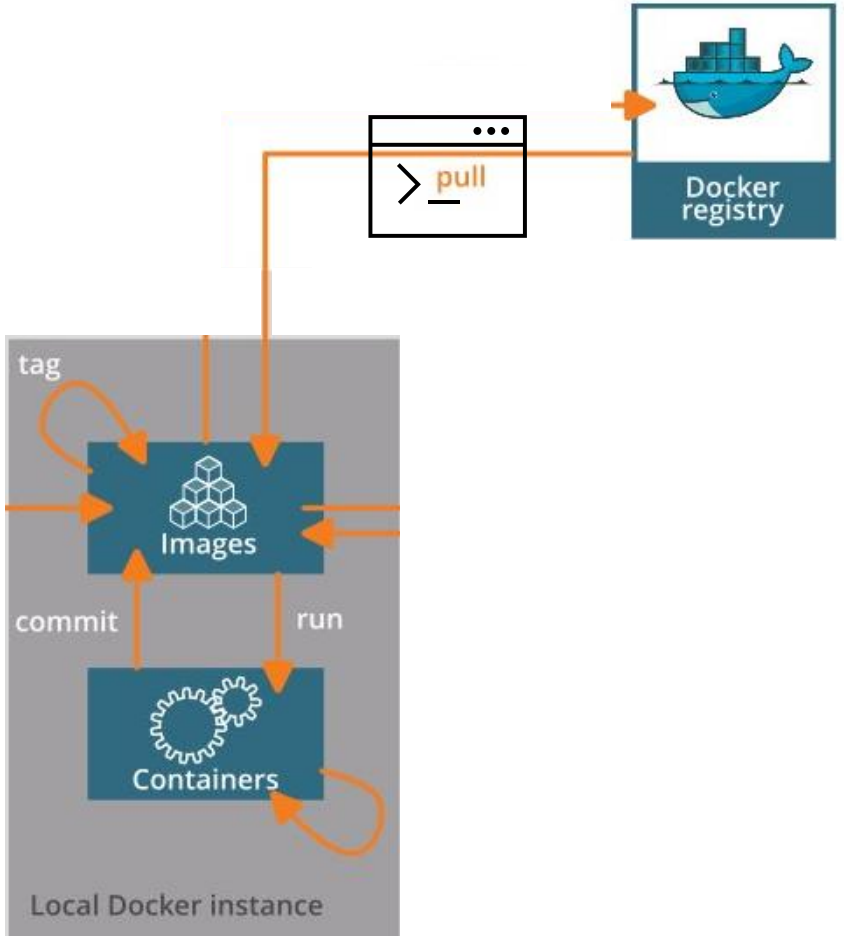
Digest: sha256:747d2dbbaaee995098c9792d99bd333c6783ce56150d1b11e333bbceed5c54d7
Status: Downloaded newer image for ubuntu:latest
```

  - Example: Get a specific version

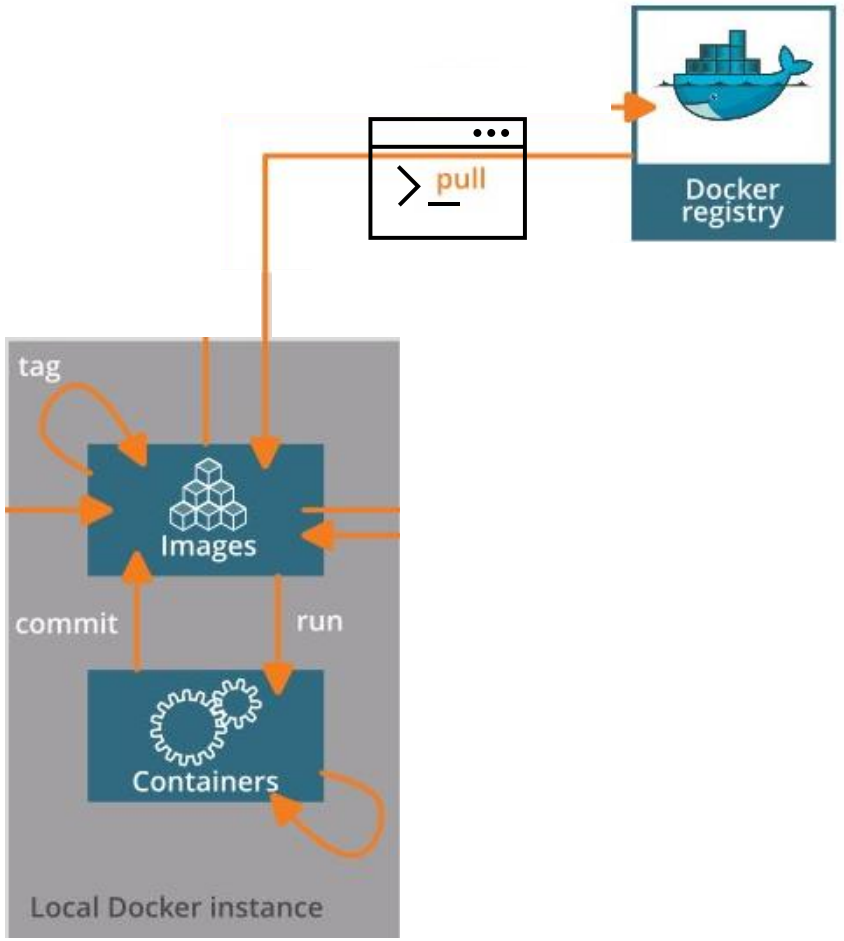
```
$ docker pull ubuntu:18.04

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 Docker hub
  - 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

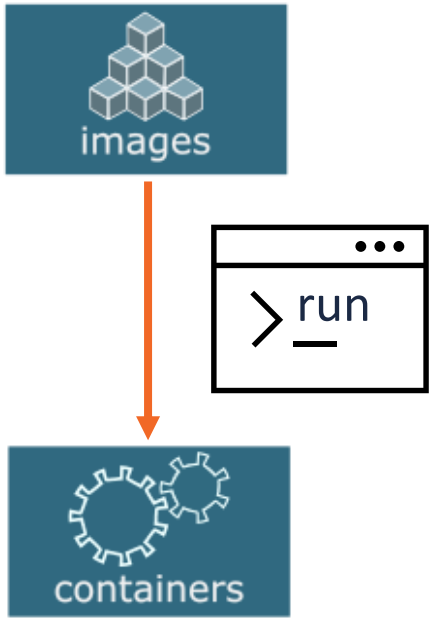
```
$ docker images
```

```
$ 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

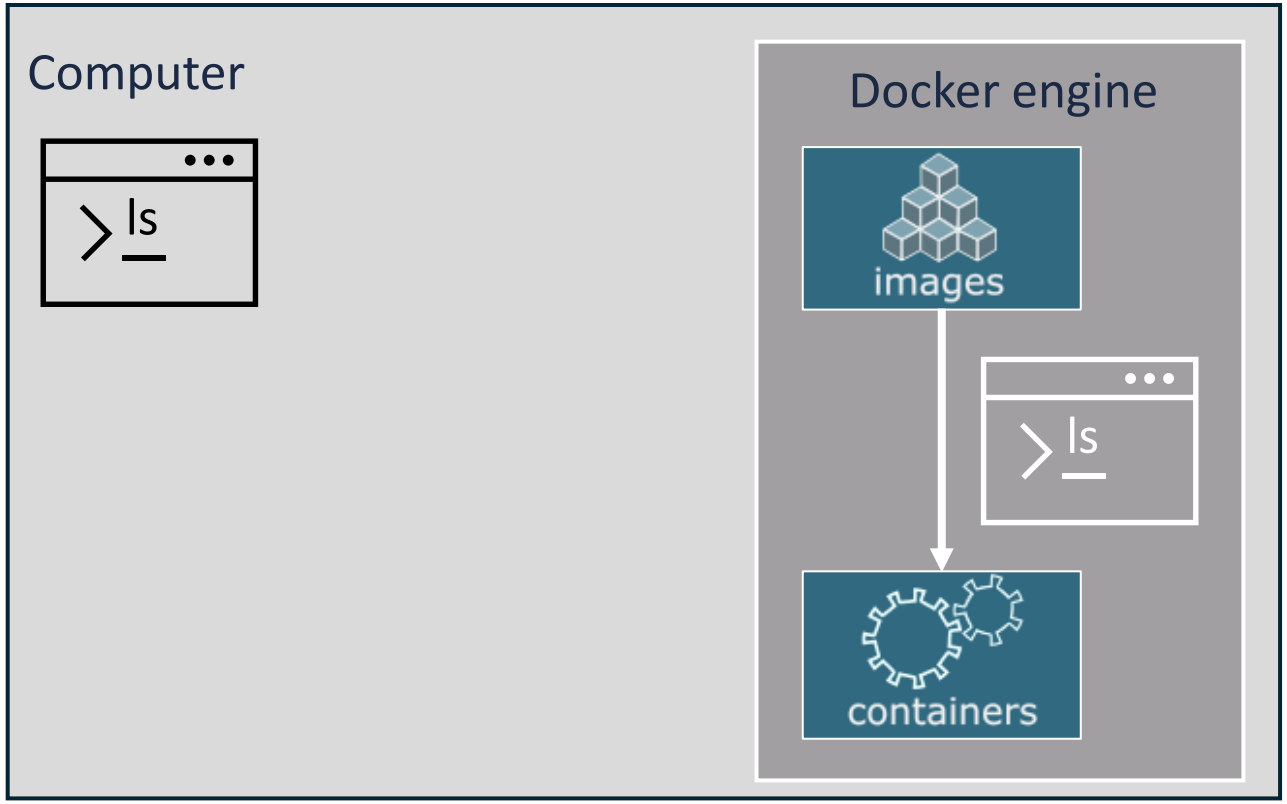
You can execute any program/command that is stored inside the image.

- 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
```

Check the name of your container by checking the process status
- Challenge: How do you list running containers?

Practice time:

- Run the following without naming it:

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

Check the name of your container by checking the process status
- Challenge: How do you list running containers?

- List running containers (process status)

```
$ docker ps
```

- List all containers (whether or not running)

```
$ docker ps -a
```

Practice time:

- Run again naming the container

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

Check the name of your container by checking the process status

```
$ docker ps
$ 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
```

- Why are IDs and Names useful for?

Practice time:

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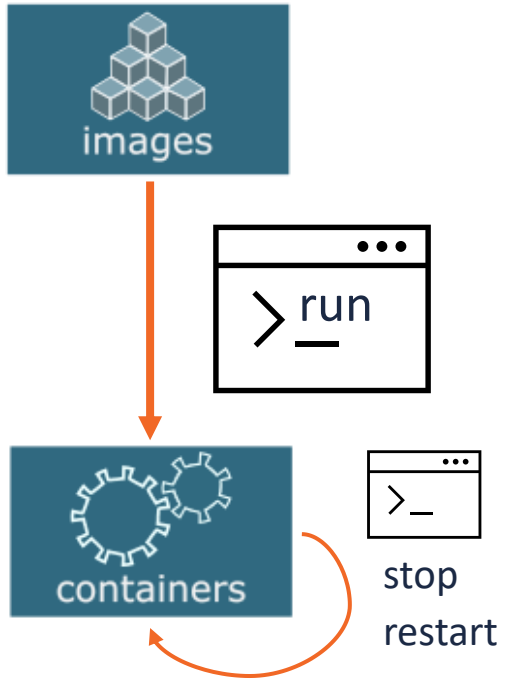
- Why are IDs and Names useful for?
  - Stop a container
  - Restart a container



Tagging

- Define image Name and Version!

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

Let’s try to do it!

Tagging

- Define image Name and Version!

```
docker tag <image ID> <container: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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```

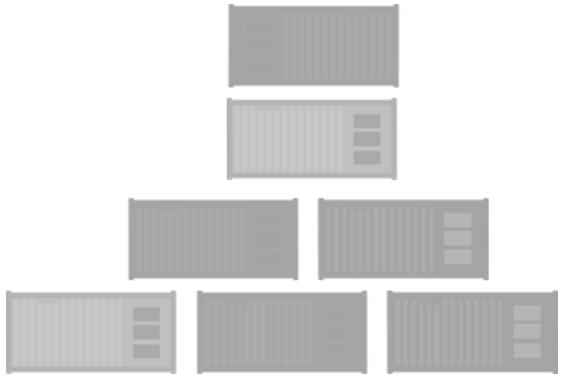
- Name an image
  - Define the version of an image (docker tag <image ID> …..)

```
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

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

```
$ docker system df
```



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

My_image

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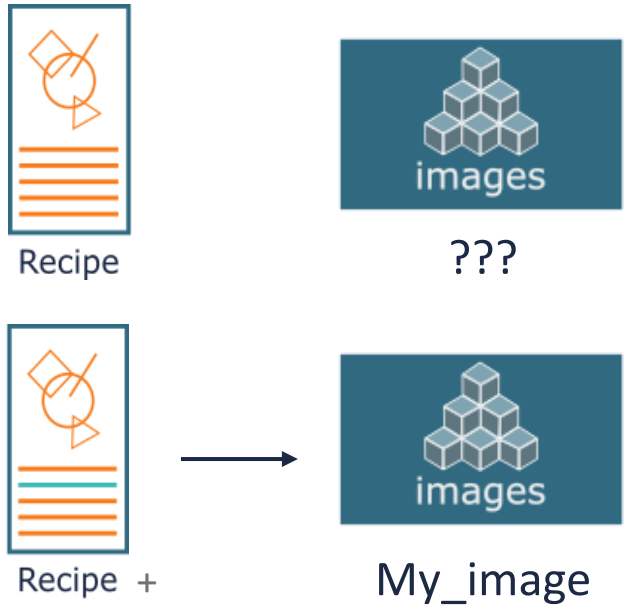

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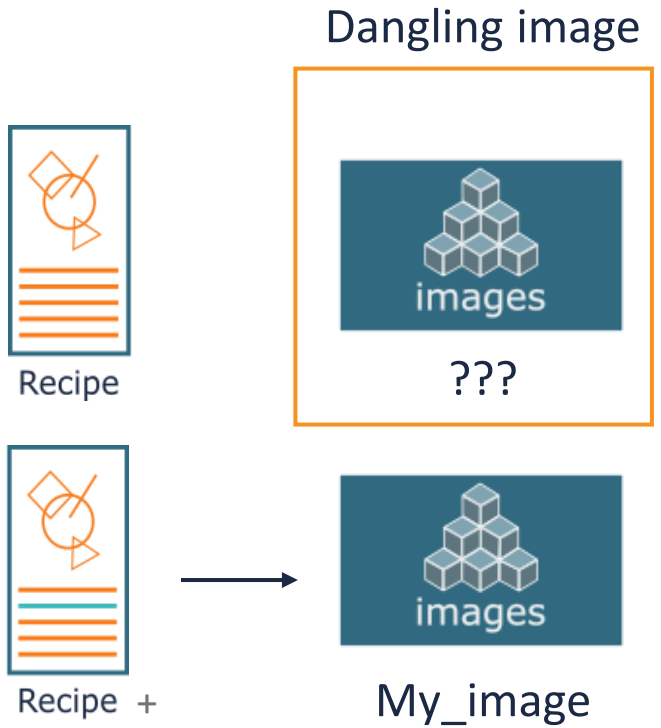

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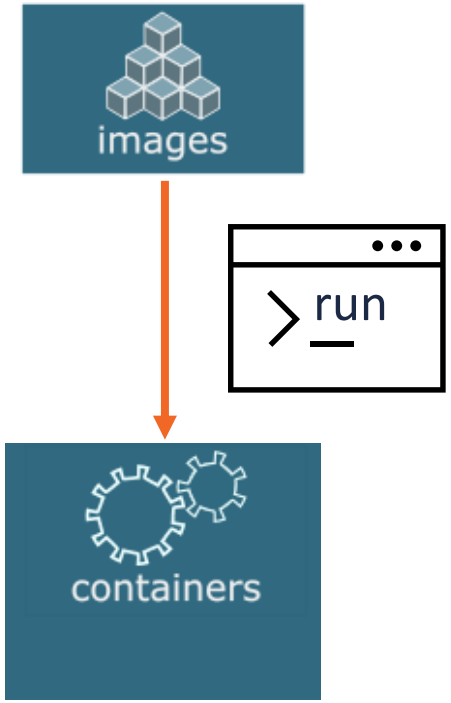

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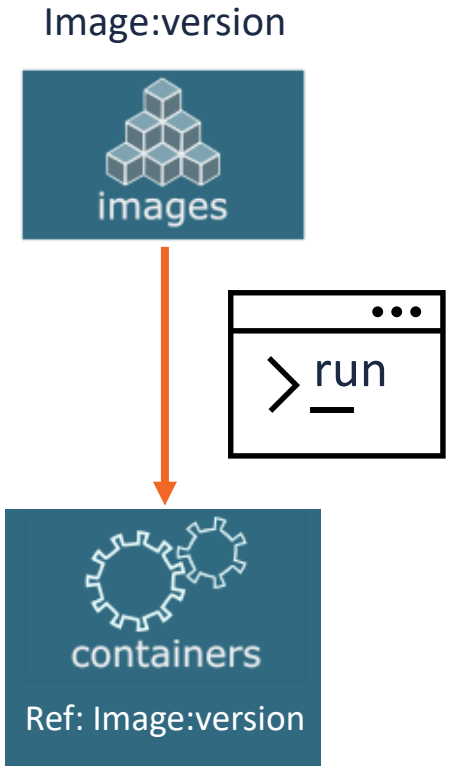

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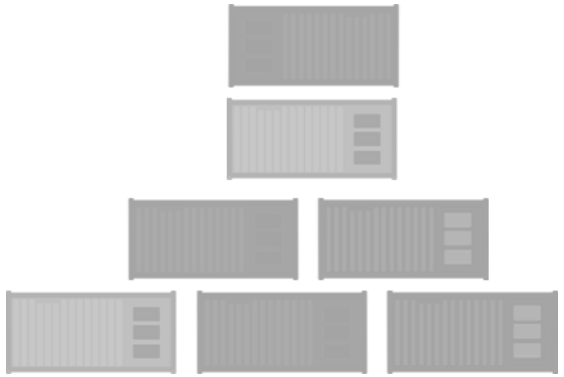


- Clean up
  - Remove (rm)
    - Specify
      - Image
      - Container

```
$ 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 –f <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:
  - Enter the container and interact:
    - docker run –it <image> <command>
    - dokcer run –it –rm <image> <command>
  - Execute a command in a running container
    - dockcer exec <containerr>

ACTIVITY TIME:

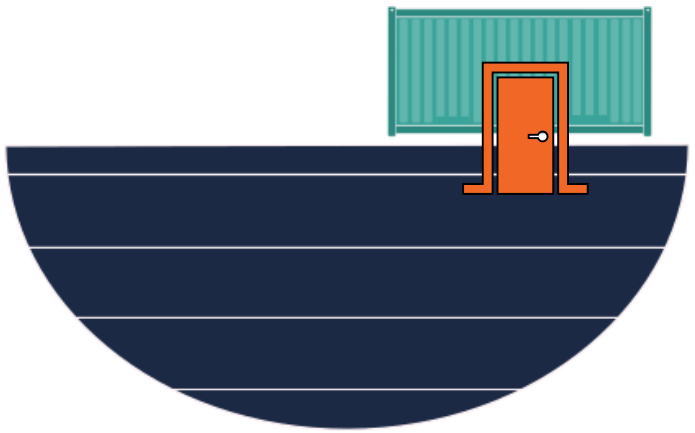
- Activity 1.1
  - Get the data (https://github.com/vibbits/containers-workshop/)
  - You will need fastqc
    - check all your images
    - Pull image if needed
  - Fastqc, version 0.11.9_cv7
    - Docker hub
  - Run fastqc –h
- Activity 1.2
  - Check for running containers
  - Remove the container
  - Run the container interactively
    - Start it with bash

- docker run –it <image> <command>
- dokcer run –it –rm <image> <command>

Docker a closed environment

Docker a closed environment

- Mounting volumes
- Using Ports



Volume mounting: I/O

- Container is isolated from host

Volume mounting: I/O

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

Volume mounting: I/O

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

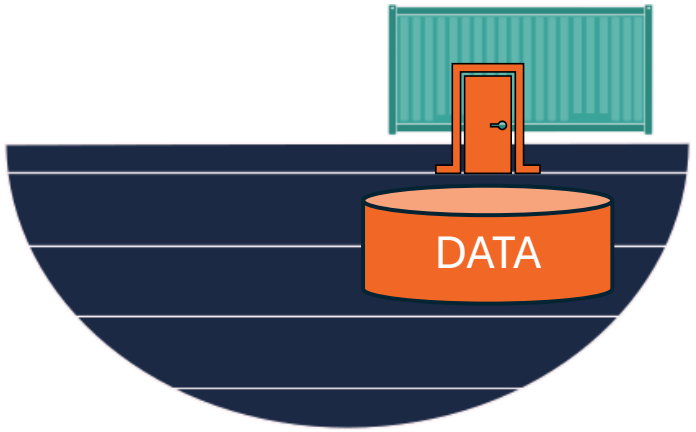
    -v /path/in/host:/path/in/container

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

  - Working directory

    -w /path/in/host

    docker run –w /path/in/host
    –volume **path/in/host/datatest:/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

- 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.

- Binding volume

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

- 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: 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.
- Host:
  - ls –ls
  - -rw-r--r-- 3 u0088910 u0088910 file1.txt
- Container:
  - ls –ls
  - -rw-r--r-- 3 root root file1.txt

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.

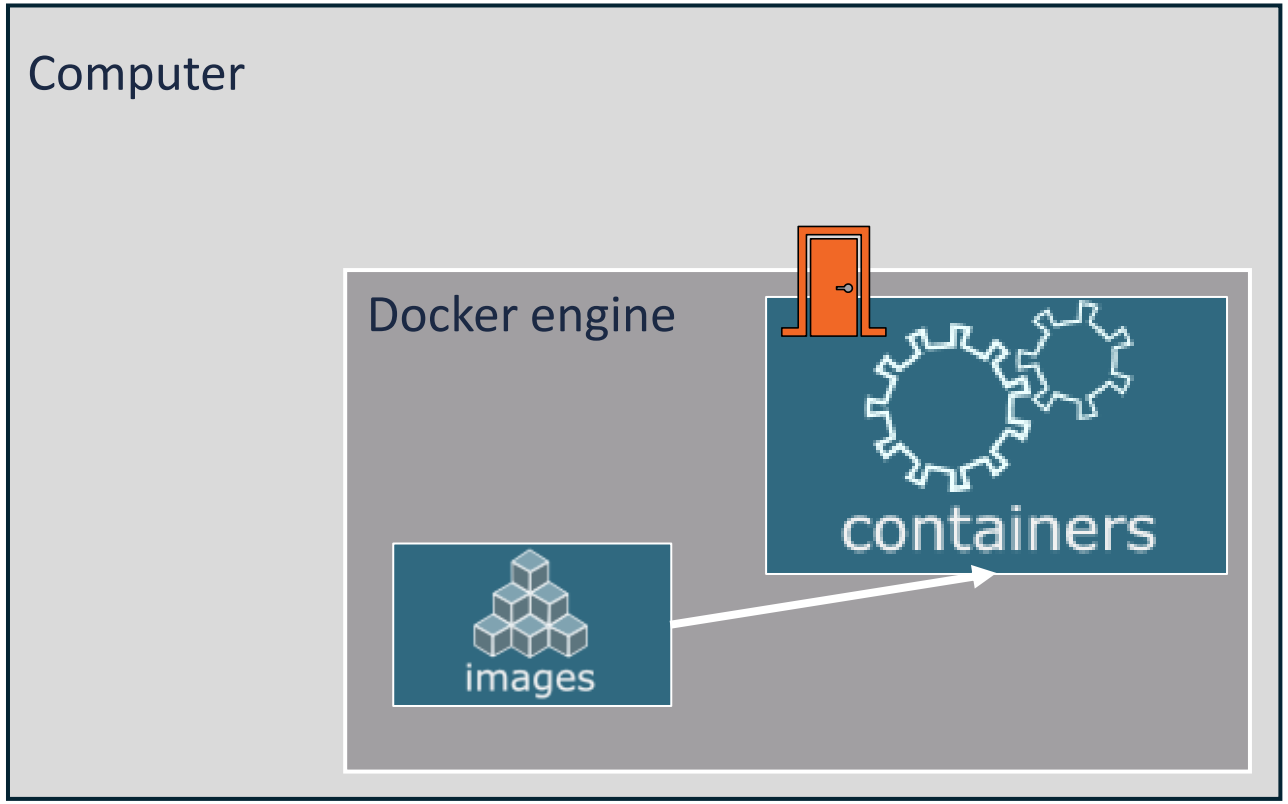
- **Extra:**
  - Can you analyze **all fastq** files using a glob-pattern (WT*.fq.gz)?
  - What do you need to change to make this work?

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

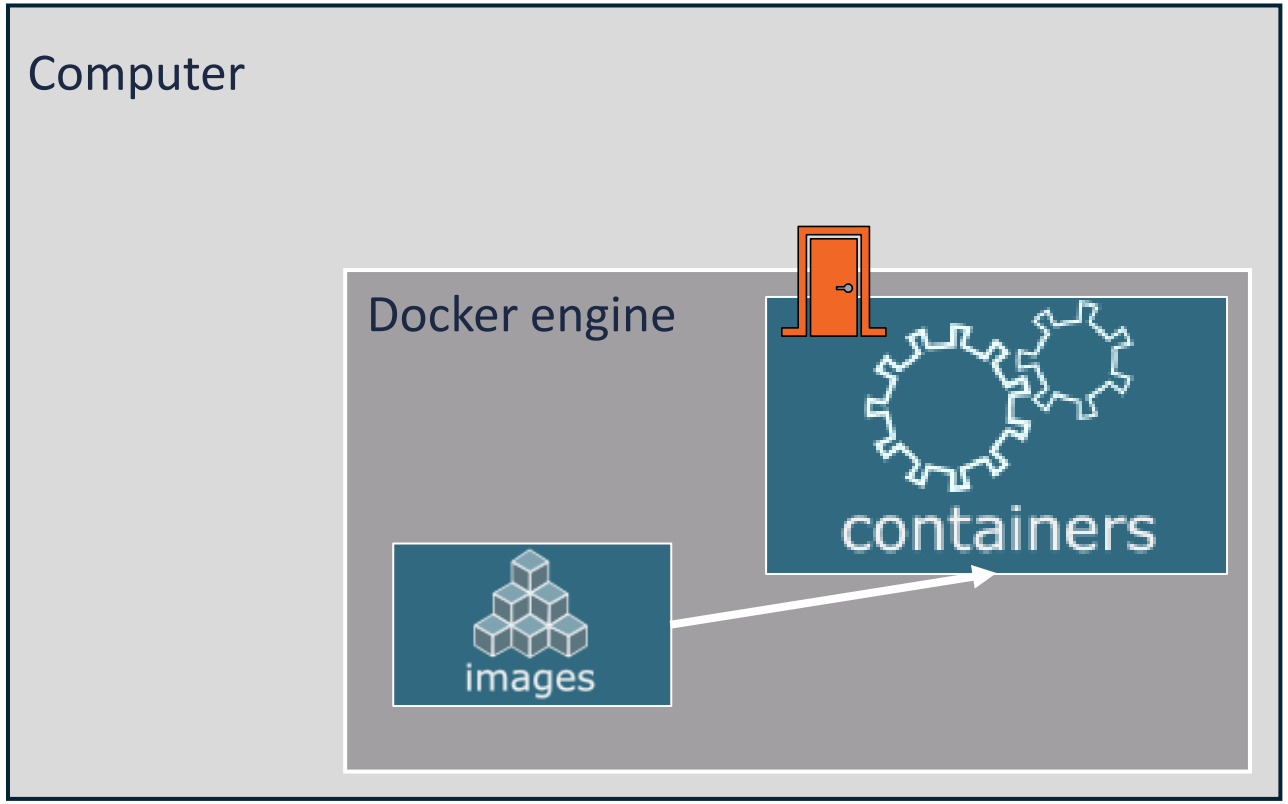
curl : Client URL

Enables communication between
the host and the server

Practice time:

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

$ curl localhost:80
```



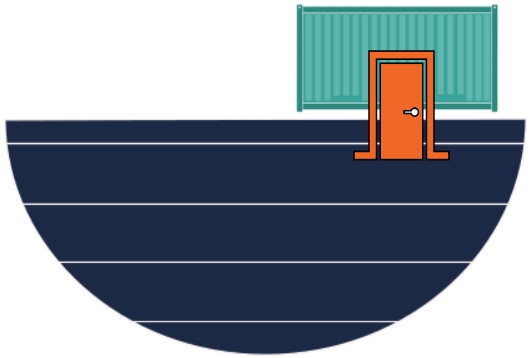
Ports

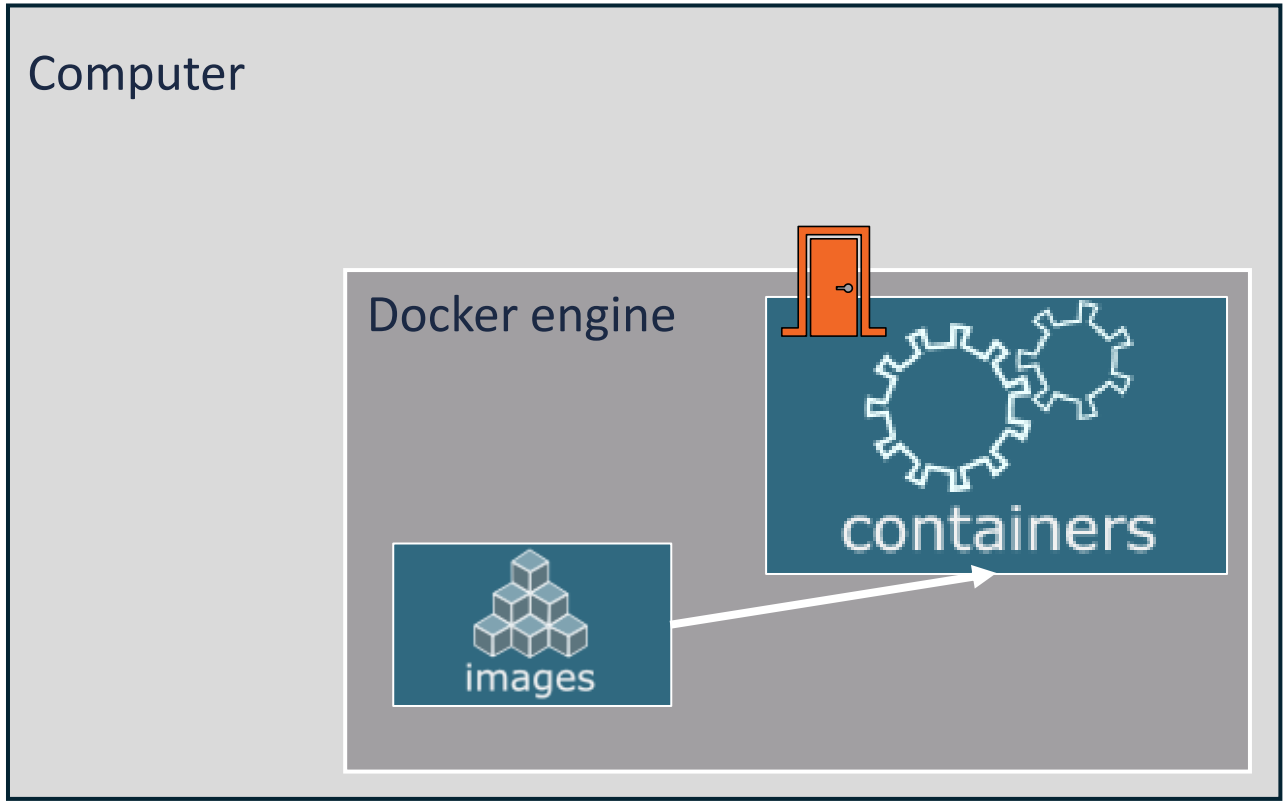
- Stablish communication with webserver

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

$ curl localhost:80
```

- Container X external environment



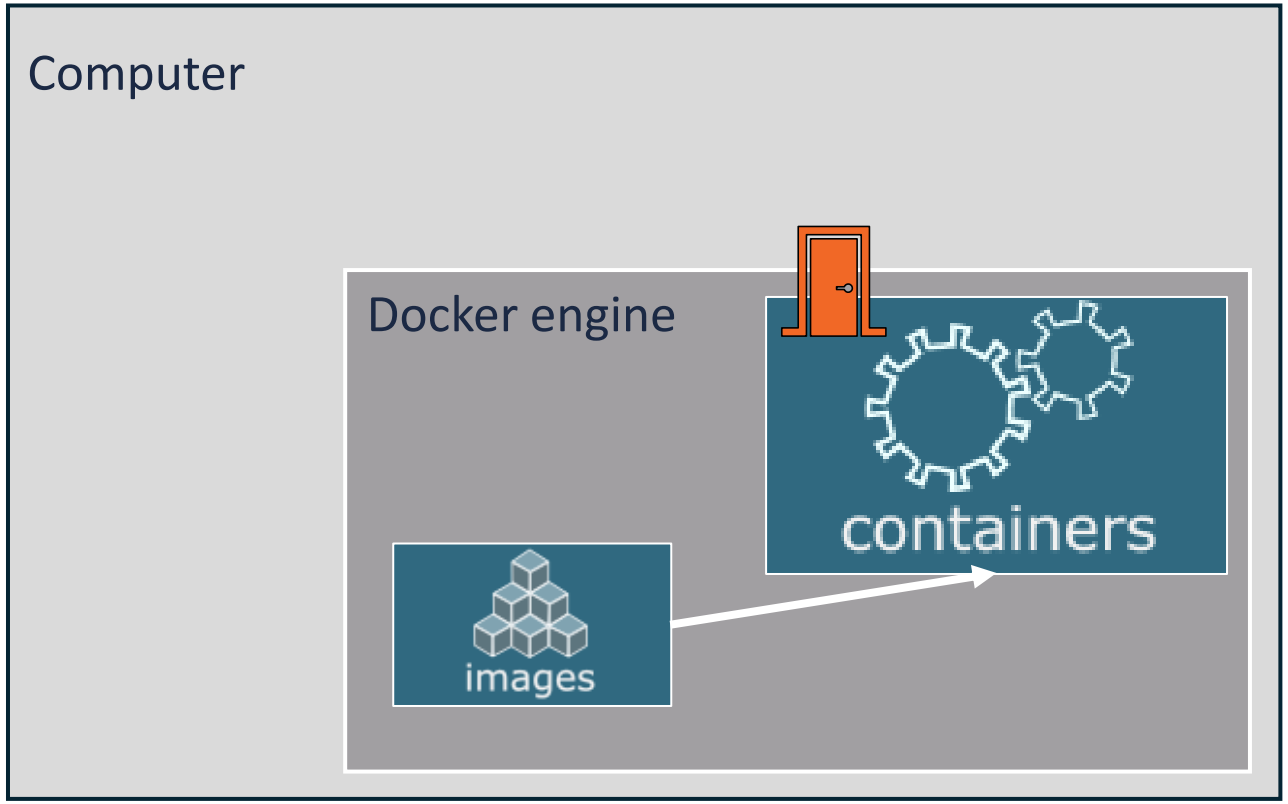


Practice time:

```
$ 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

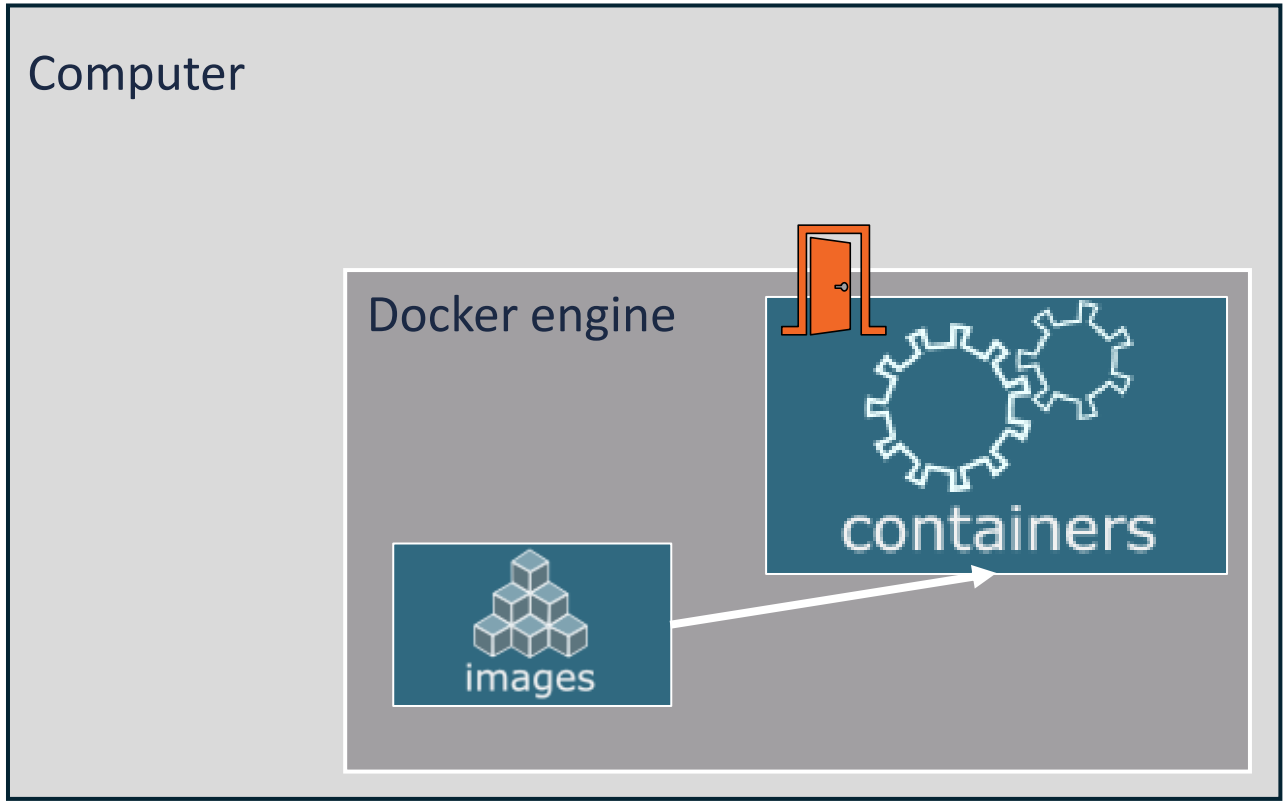
```
$ docker run --detach --name webserver nginx

$ curl localhost:80
```

- Container X external environment

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

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

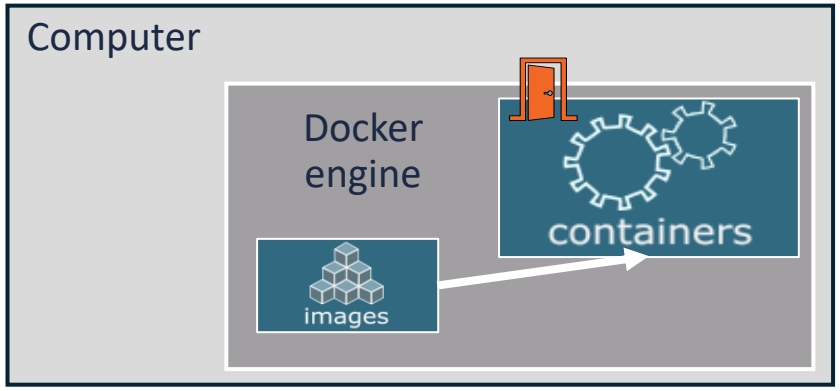


Ports

- To keep the door open

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

```
$ curl localhost:80
```



Ports

- To keep the door open

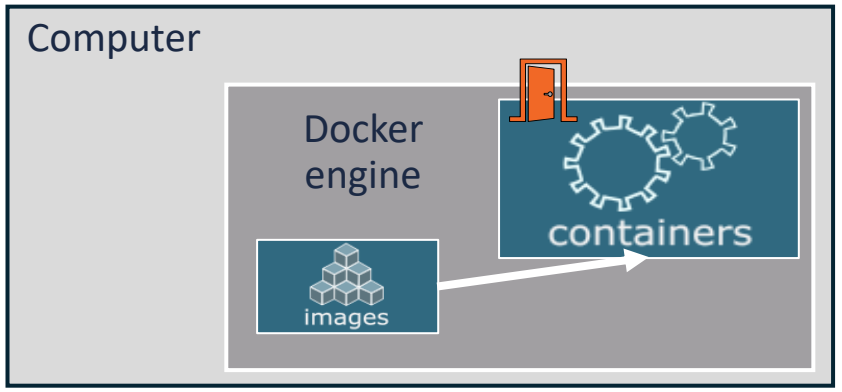
```
$ docker run --detach --name webserver --publish 80:80 nginx

$ 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

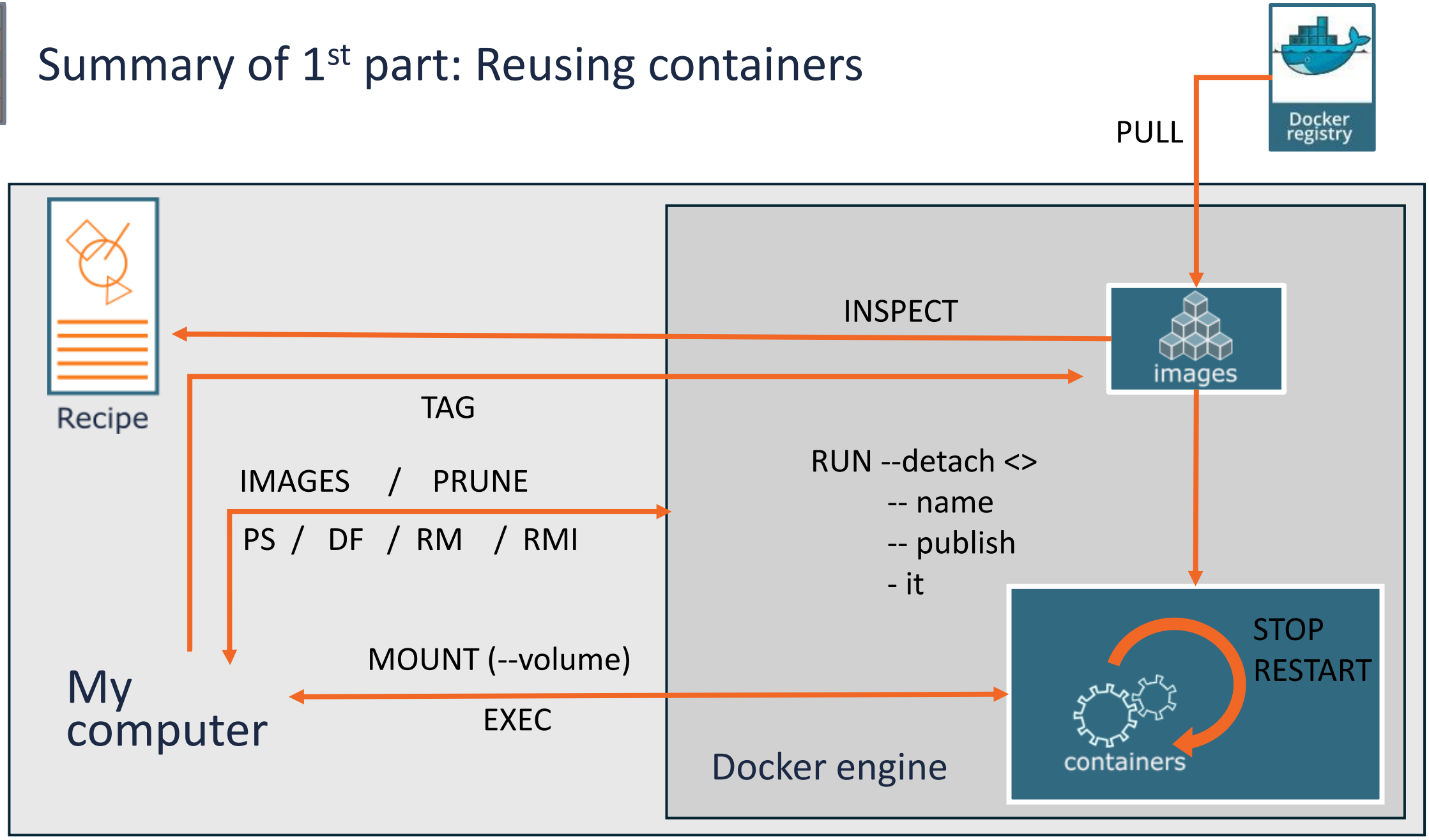
- Inspect the image biocontainers/fastqc:0.11.9_cv7

- Extract the working directory (WorkingDir) using grep.

HINT:

```
cmd | grep “keyword”
```

Summary of 1st part: Reusing containers



Building your own docker image

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.

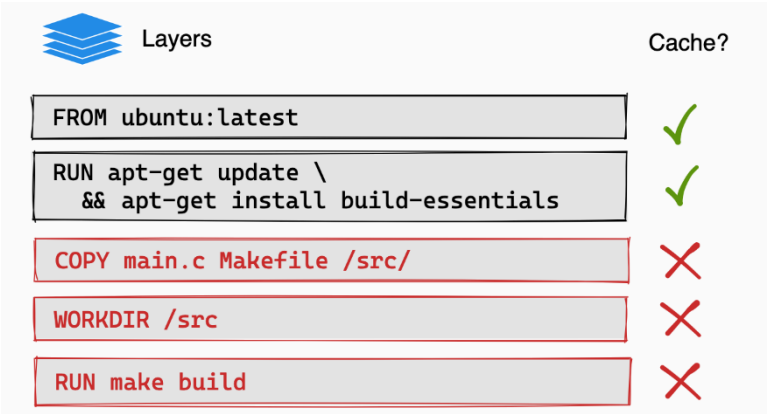
```
FROM ubuntu:18.04

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

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.

What do you expect your container to do?

Makes easier to maintain the container.

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

•Published: November 10, 2020
•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

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

ACTIVITY TIME:

https://github.com/vibbits/containers-workshop/blob/main/exercises/02_building_dockerfiles.md

- Exercise 5.2
  - You need to pull jupyter/scipy-notebook:python-3.11.5
  - Once you have it, run the script from outside the container ***codereppy_min_batch.py***

Reach out to your neighbour(s) in case you need help.

```
docker run --detach --rm -v ./data:/home/jovyan/ jupyter/scipy-notebook:python-3.11.5 python ./data/codereppy_min_batch.py
docker run --detach --rm -w /data -v ./data:/data jupyter/scipy-notebook:python-3.11.5 python ./data/
docker run --detach --rm -w /data -v ./data:/data jupyter/scipy-notebook:python-3.11.5 python codereppy_min_batch.py

docker run -it --rm -w /data -v ./data:/data jupyter/scipy-notebook:python-3.11.5 bash || python codereppy_min_batch.py
docker run -it -u root -w /data -v ./data:/data jupyter/scipy-notebook:python-3.11.5 bash || python codereppy_min_batch.py
```

ACTIVITY TIME:

https://github.com/vibbits/containers-workshop/blob/main/exercises/02_building_dockerfiles.md

- Exercise 6
  - You “found” a Dockerfile on github – now in the docker folder
    - Dockerfile.deploy-cloud
  - Try to build the image
  - Run the Docker image – what does the container do?
  - Test the container
  - You need the Python script test_query.py which is in the data folder

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

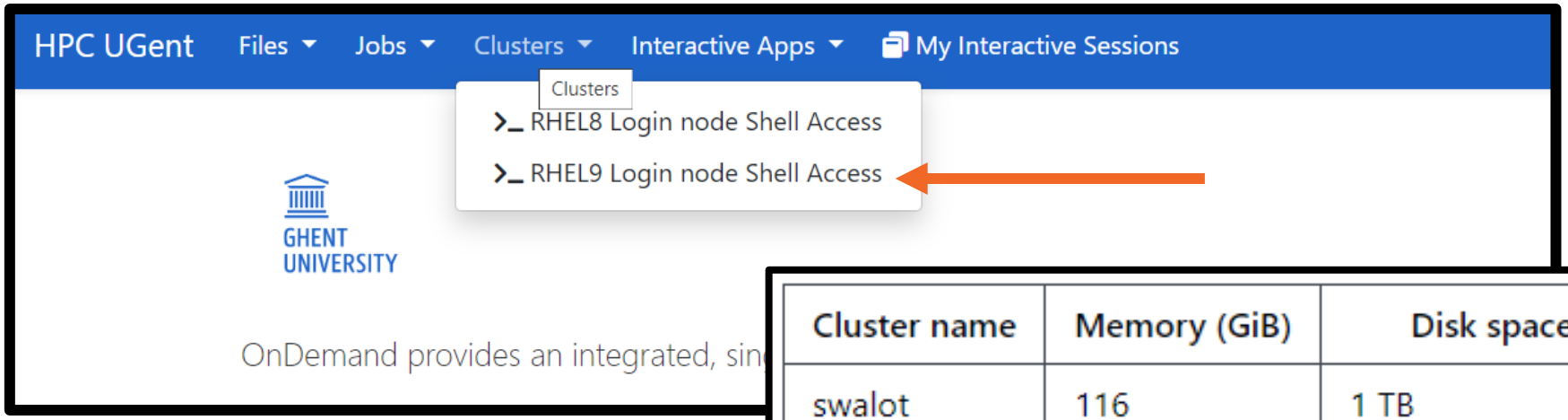
Short intro to HPC

preparing for Apptainer

VIB technologies

ELIXIR BELGIUM

Ugent : Ondemand - https://login.hpc.ugent.be



UGent TIER1 clusters

Cluster name	Memory (GiB)	Disk space	GPU
swalot	116	1 TB	-
skitty	177	1 TB + 240 GB SSD	-
victini	88	1 TB + 240 GB SSD	-
joltik	256	800 GB SSD	4 NVIDIA V100
doduo	250	180 GB SSD	-
accelgor	500	180 GB SSD	4 NVIDIA A100
donphan **	738	1.6 TB NVME	1 shared NVIDIA Ampere A2
gallade	940	1.5 TB NVME	-

VSC - UGent

Filesystems specifics

Filesystem name	Intended usage
$VSC_HOME	Home directory, Not the entry point to the system, same as Tier2
$VSC_SCRATCH	Entry point to the system
$VSC_DATA	Long-term storage of large data files
/dodrio/scratch/projects/starting_2023_001/	Temporary fast storage of 'live' data for calculations

** Storage space for a group of users (Virtual Organisation or VO for short) can

Usually where you arrive when login in
Not much space
Not for running analysis

More space
Where you run analysis (input/output)

Long term storage
Archive also
Large files

UGent TIER1

Filesystem name	Intended usage	Total storage space	Personal storage space	VO storage space **
$VSC_HOME	Home directory, Not the entry point to the system, same as Tier2	?	3GB (fixed)	✗
$VSC_SCRATCH	Entry point to the system	?	3GB (fixed)	✗
$VSC_DATA	Long-term storage of large data files	?	Depend of you account(Leuven/Gent, see above)	✗
/dodrio/scratch/projects/starting_2023_001/	Temporary fast storage of 'live' data for calculations	?	10TB	?

** Storage space for a group of users (Virtual Organisation or VO for short) can be increased significantly on request.

•Source : https://docs.vscentrum.be/gent/tier1_hortense.html#system-specific-aspects

UGent TIER2

Filesystem name	Intended usage	Total storage space	Personal storage space	VO storage space (*)
$VSC_HOME	Home directory, entry point to the system	51 TB	3GB (fixed)	✗
$VSC_DATA	Long-term storage of large data files	1.8 PB	25GB (fixed)	250GB
$VSC_SCRATCH	Temporary fast storage of 'live' data for calculations	1.9 PB	25GB (fixed)	250GB
$VSC_SCRATCH_ARCANINE	Temporary very fast storage of 'live' data for calculations (recommended for very I/O-intensive jobs)	70 TB	(none)	upon request
(*) Storage space for a group of users (Virtual Organisation or VO for short) can be increased significantly on request.				

•Source : https://docs.vscentrum.be/en/latest/gent/tier2_hardware.html?highlight=VSC_DATA#shared-storage

KULeuven TIER2

Filesystems specifics

Filesystem name	Intended usage	Total storage space	Personal storage space	VO storage space (*)
$VSC_HOME	Home directory, entry point to the system	?	3GB (fixed)	❌
$VSC_DATA	Long-term storage of large data files	?	75GB (fixed)	❌
$VSC_SCRATCH	Temporary fast storage of 'live' data for calculations	?	500GB	?

•Source https://docs.vscentrum.be/en/latest/leuven/tier2_hardware/kuleuven_storage.html?highlight=VSC_DATA#ku-leuven-storage

KULeuven – TIER2 clusters

Clsuters specifics at UGent - VSC

On top of the filesystem, each clusters will have different computational powers, therefore, depending on your needs, you can choose the one that most suits you.

Cluster name	Memory (GiB)	Disk space	GPU
swalot	116	1 TB	-
skitty	177	1 TB + 240 GB SSD	-
victini	88	1 TB + 240 GB SSD	-
joltik	256	800 GB SSD	4 NVIDIA V100
doduo	250	180 GB SSD	-
accelgor	500	180 GB SSD	4 NVIDIA A100
donphan **	738	1.6 TB NVME	1 shared NVIDIA Ampere A2
gallade	940	1.5 TB NVME	-

** debugging cluster (Used for debugging and training)

Using KULeuven ondemand:
https://ondemand.hpc.kuleuven.be

VSC - UGent

Submission command

- qsub submission_script.sh
- sbacth submission_script.sh

```
#!/bin/bash
#SBATCH --job-name= Apptainer-donphan
#SBATCH --output= raboti_vistro.out
#SBATCH --ntasks= 1
#SBATCH --time= 1:00:00
#SBATCH --mem-per-cpu= 16G
#SBATCH --partition= cluster/dodrio/gpu_rome_a100
#SBATCH --gres= gpu:1
#SBATCH --cpus-per-task= 16
#SBATCH --error= raboti_vistro.%j.err
#SBATCH --account= starting_2023_001

module swap cluster/dodrio/gpu_rome_a100
module load  scikit-image/0.19.3-foss-2022a
module load  n2v/0.3.2-foss-2022a-CUDA-11.7.0

python
/dodrio/scratch/users/vsc33625/00_02_prediction_d
enoising_batch.py
```

VSC - UGent

Commands in the HPC

- `module avail` : list all available modules
- `module spider <key word>` : search specific modules
- `module swap cluster/donphan` : Swap to specific cluster

Checking your JOB submission

- `squeue` : check status

- `Scancel <job ID>` : kill a job

For more: https://docs.vscentrum.be/jobs/job_management.html

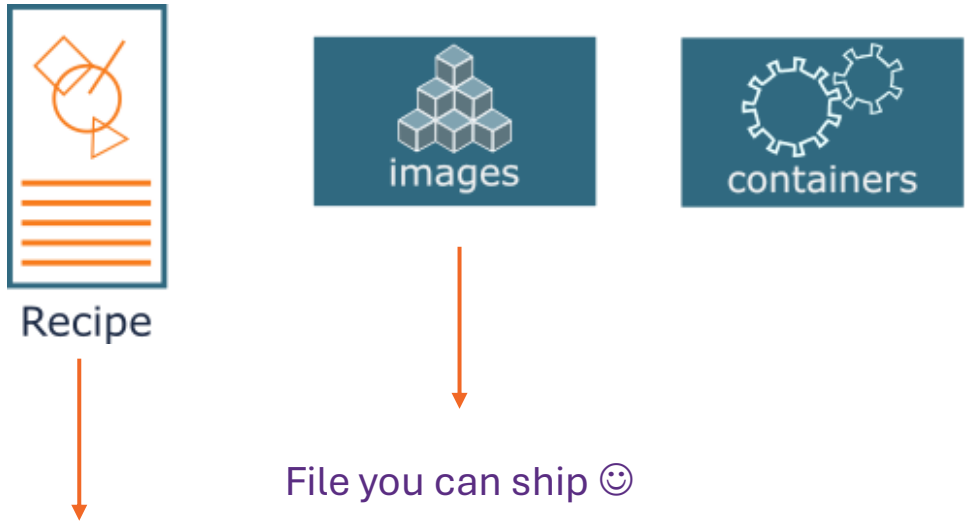
Status	Code
COMPLETED	CD
COMPLETING	CG
FAILED	F
PENDING	PD
PREEMPTED	PR
RUNNING	R
SUSPENDED	S
STOPPED	ST

https://curc.readthedocs.io/en/latest/running-jobs/squeue-status-codes.html

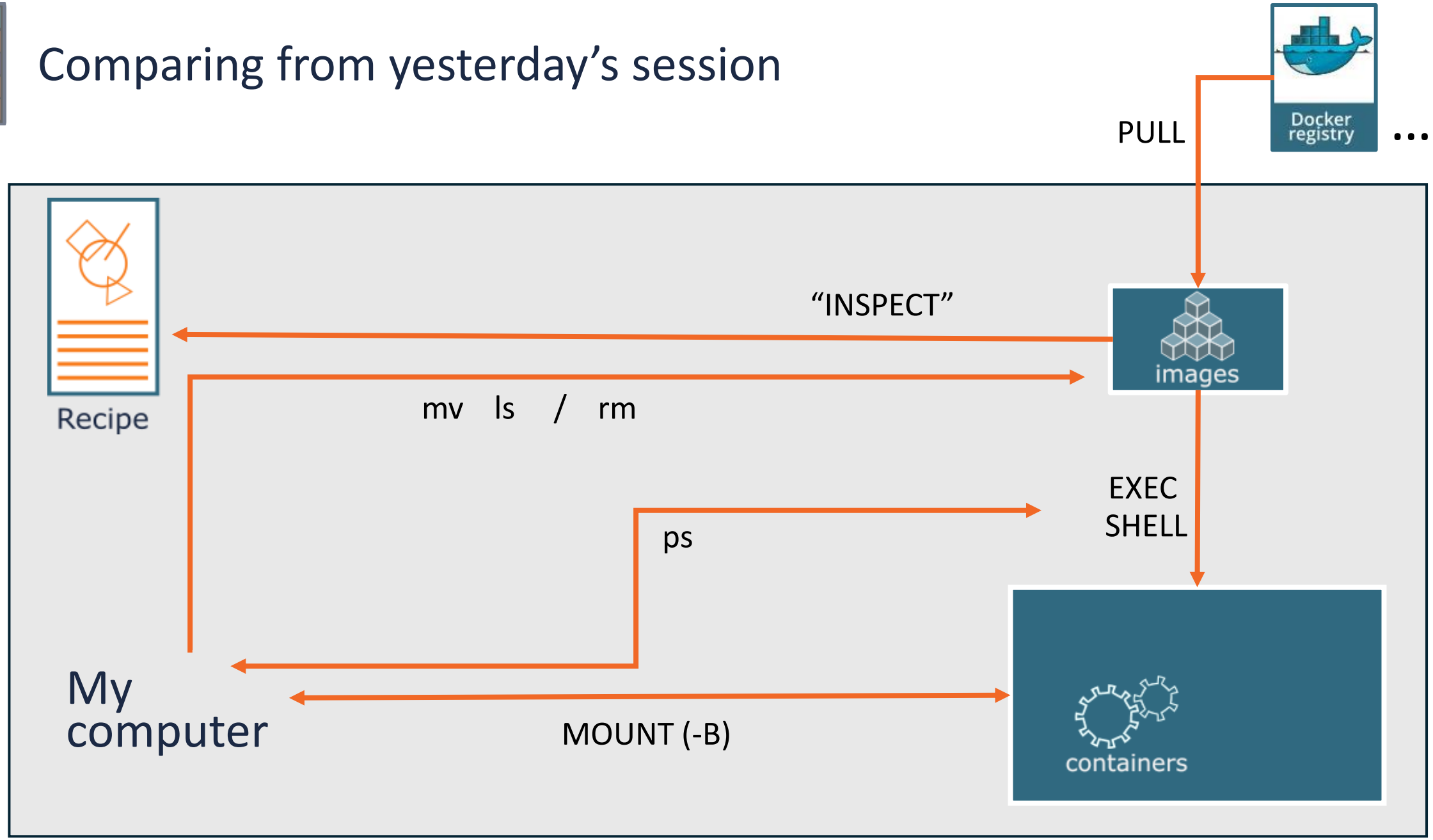
Introduction to Apptainer for reproducible analysis

How does it work?

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

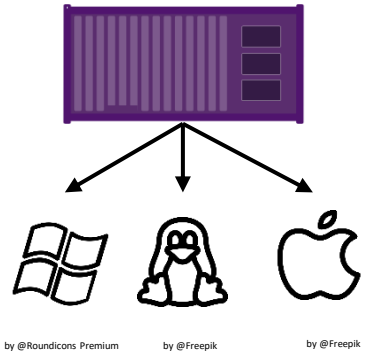


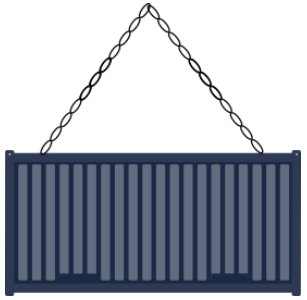
Comparing from yesterday's session



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
```

Analysis with FASTqC

```
$ 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

$ $VSC_SCRATCH > git clone https://github.com/vibbits/containers-workshop

$ run > bash data/downl-data.sh

$ run fastqc via singularity image in at least one file example.
```

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

There are folders like this /staging/leuven/stg007/vrc/…

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

  ...