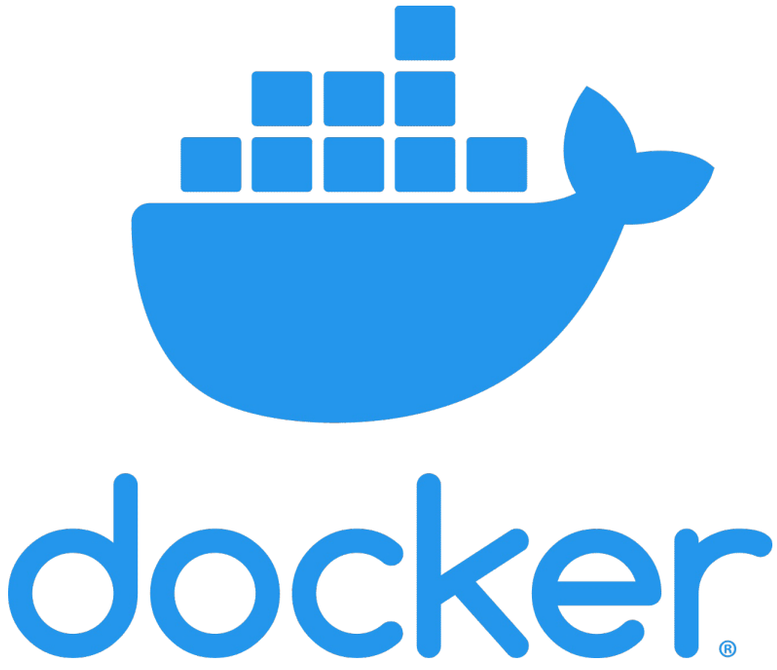
Making self-contained, distributable projects with



Singularity

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What is Docker?

- Standardized packaging for software and dependencies
- Docker lets you create and run applications securely isolated in a container, packaged with all its dependencies and libraries.

Docker in lifescience

Docker containers can be used to allow others to reproduce a complete analysis:

> To further support reproducibility, we bundled all tools and dependencies into one Docker container available on DockerHub [19]. docker run executes the aforementioned Makefile inside the container.

(click here to see the Dockerfile)

```
docker run metagenomics/2015-biogas-cebitec
```

Bremges et al GigaScience (2015) 4:33, doi:10.1186/s13742-015-0073-6

Docker in lifescience

Docker can also be used to define software environments and settings for benchmarking studies

CAMI Challenge: an independent evaluation of several tools in the field of metagenomics

> ... we defined standards for submitting the software itself, along with parameter settings and required databases and implemented them in Docker container templates...

Sczyrba et al Nature Methods (2017) 14:1063–1071, doi.org/10.1038/nmeth.4458

Docker in lifescience

Docker can also be used to define software environments and settings for benchmarking studies

2nd CAMI Challenge

> For reproducibility, participants could submit a Docker container containing the complete workflow, a bioconda script or a software repository with detailed installation instructions...

Meyer et al Nature Methods (2022) 19:429-440, https://doi.org/10.1038/s41592-022-01431-4

Docker nomenclature

- A Docker file is a recipe used to build a Docker image
- A Docker image is a standalone executable package of software
- A Docker container is a standard unit of software run on the Docker Engine.
- Docker Hub is an online service for sharing docker images

Images and containers

Example: Use a different OS

Check OS on local machine

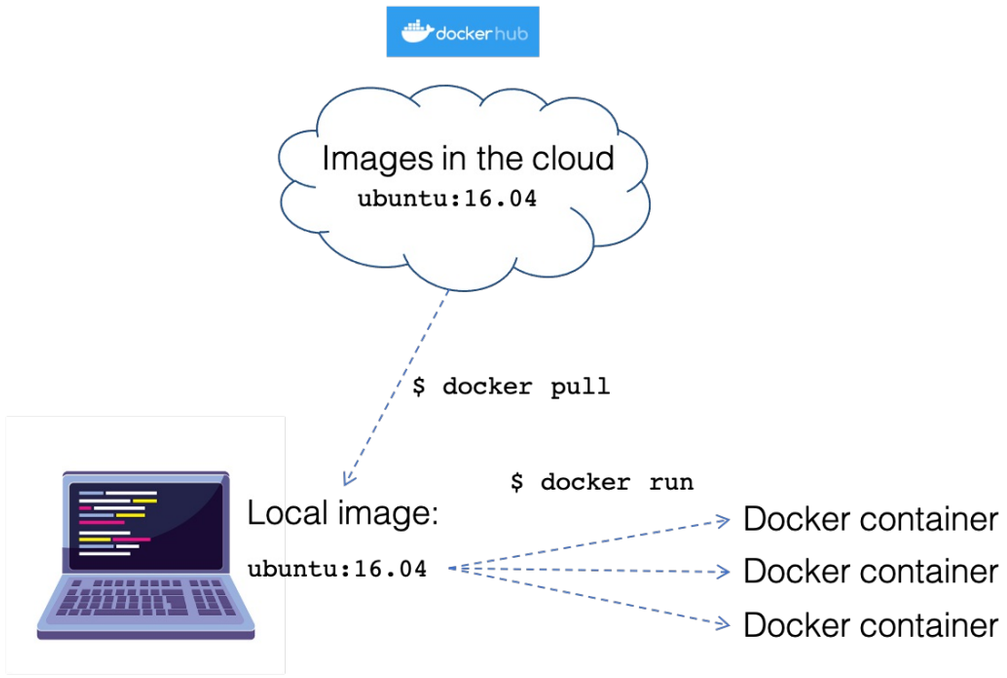
```
$ uname -a
Darwin johnsmbp.local 19.6.0 \
Darwin Kernel Version 19.6.0: \
Tue Jan 12 22:13:05 PST 2021; \
root:xnu-6153.141.16~1/RELEASE_X86_64 x86_64
```

Pull Ubuntu (Linux) image

```
$ docker pull ubuntu:16.04
16.04: Pulling from library/ubuntu
22dc81ace0ea: Pull complete
...
Digest: sha256:e348fbbea0e0a0e73ab0370de151e7800684445c509d46195aef73e090
Status: Downloaded newer image for ubuntu:16.04
```

Run a container and check OS version

```
$ docker run -it ubuntu:16.04
root@407b0fd13fe5:/# uname -a
Linux 407b0fd13fe5 4.9.60-linuxkit-aufs #1 SMP Mon Nov 6 16:00:12 UTC
2017 x86_64 x86_64 x86_64 GNU/Linux
```



Mounting volumes

```
$ docker run -it -v $PWD/data:/home/data ubuntu:16.04
```

Local project directory:

```
$ ls project/

l- doc/
l
l- data/
l  l- raw_external/
l  l- raw_internal/
l  l- meta/
l
l- code/
l- notebooks/
l
l- intermediate/
l- scratch/
l- logs/
l
l- results/
l  l- figures/
l  l- tables/
l  l- reports/
l
l- Snakefile
l- config.yml
l- environment.yml
l- Dockerfile
```

Docker image file system

```
$ ls /

l- bin/
l- boot/
l- dev/
l- etc/
l- home/
l  l- data/ # data folder mounted under home/
l     l- raw_external/
l     l- raw_internal/
l     l- meta/
l- lib/
l- lib64/
l- media/
l- opt/
l- proc/
l- root/
l- run/
l- sys/
l- tmp/
l- usr/
l- var/
```

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What can I use Docker for?

- As an advanced environment manager

```
docker run -it -v $PWD:/home my_image /bin/bash
```

- To package your code with the environment it needs

```
docker run \
-v $PWD/data:/home/data \
-v $PWD/results:/home/results \
my_image snakemake report.pdf
```

- To package a whole workflow with environment, code and data (e.g. to accompany a manuscript).

```
docker run \
-v $PWD/results:/home/results \
my_image snakemake report.pdf
```

- and much more...

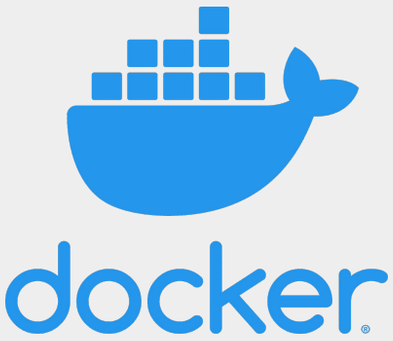
What is Singularity?

an open source container platform suitable for HPC clusters

https://sylabs.io/guides/latest/user-guide/

> Singularity was created to run complex applications on HPC clusters in a simple, portable, and reproducible way.

Docker vs. Singularity

	
runs as a daemon process with superuser privileges	runs as regular user
images stored centrally	image files that you can move around. No layers!
isolates the host and container file system by default	containers have access to host file system
well supported on Mac/Linux/Windows	limited support on Mac/Windows

Questions?

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