



INSTITUT FRANÇAIS DE BIOINFORMATIQUE



Environment manager from your OS to your environment

Encapsulation levels using Conda, Docker and Singularity



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7 juillet 2023



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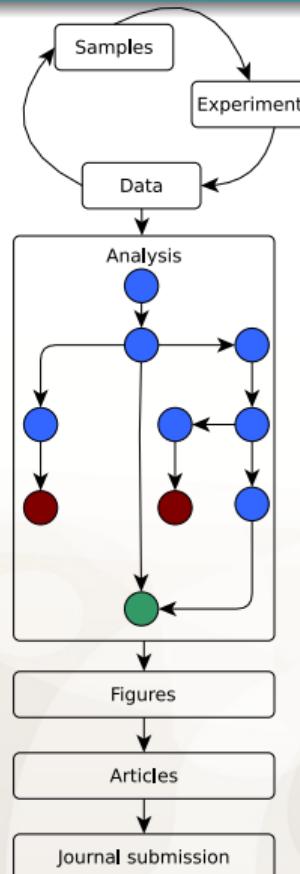


. This work is based on the IFB and I2BC formation offer

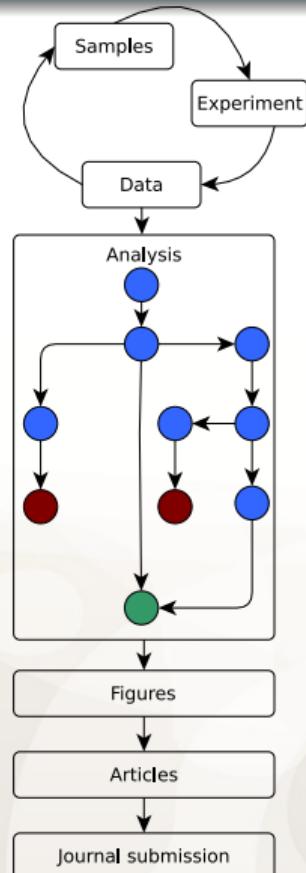
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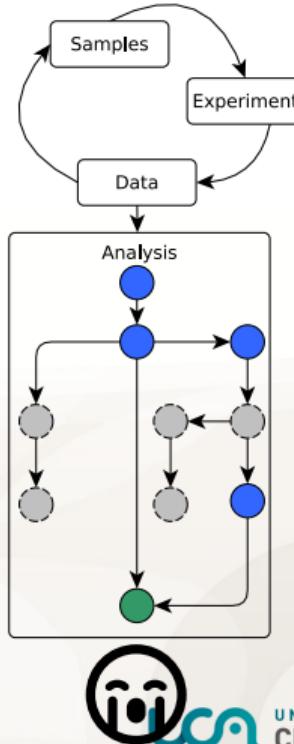
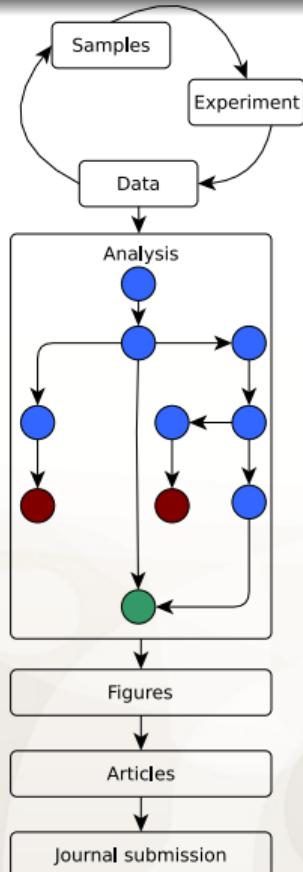
A classic use case



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A classic use case

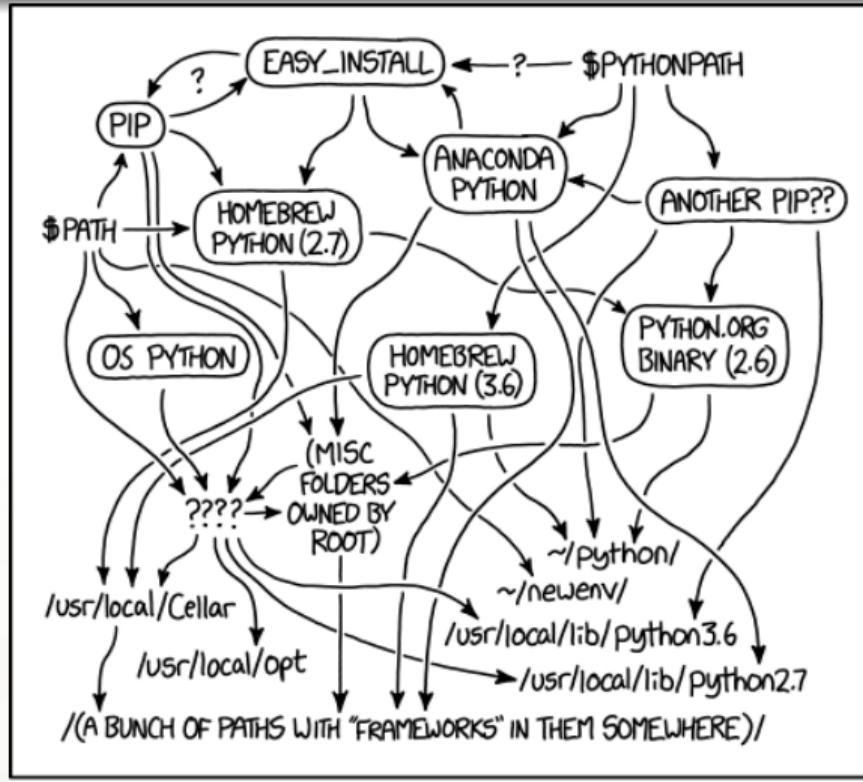
What are the changes ?

- Tool version
- Packages
- Environment variables
- OS version
- The computer
- ...

■ Tool compatibility troubles

- Python version ? 2.7, 3.8...
- Which tool version ?
- Installation without root access
- coexistence between several versions, libraries

My python env



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

Encapsulation levels

Encapsulation : capture the environment of applications (OS, packages, libraries) to control their execution

- Environment management (package manager) **CONDA**

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- Environment management (package manager) **CONDA**



- Hardware virtualisation (virtual machines)



- OS virtualisation (images and containers)

Example of R and package installation

Classical installation

- Start with a computer and a specific OS

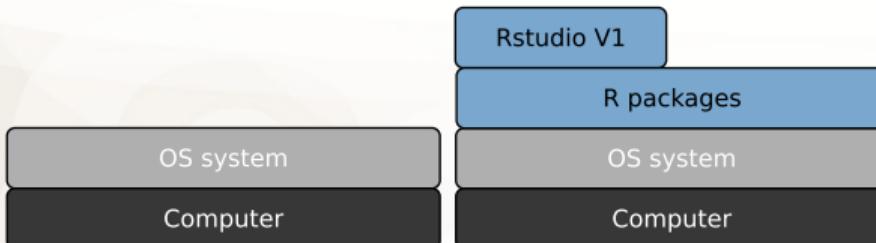
OS system

Computer

Example of R and package installation

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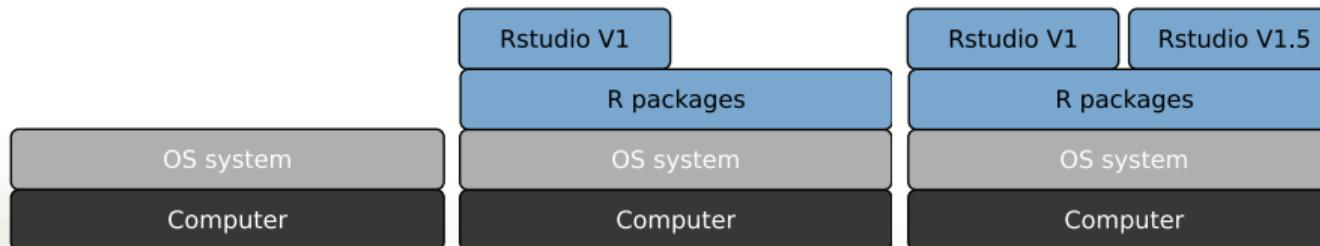
- Start with a computer and a specific OS
- Inside, we installed a new  application



Example of R and package installation

Classical installation

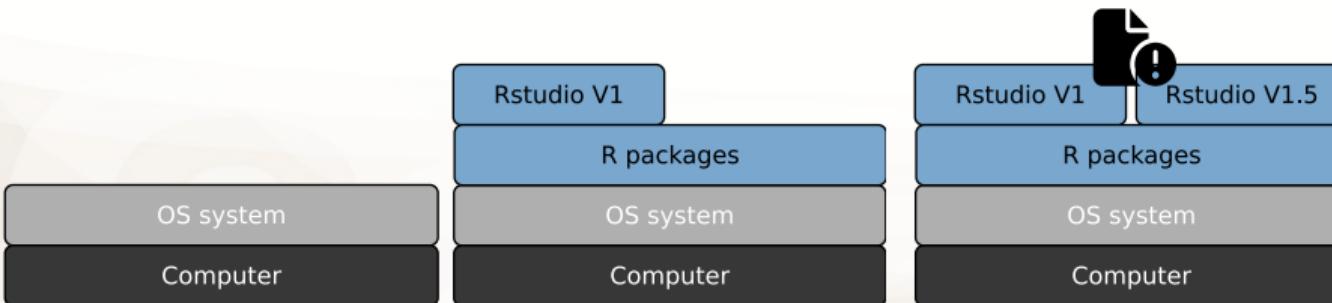
- Start with a computer and a specific OS
- Inside, we installed a new  application
-  need some dependencies



Example of R and package installation

Classical installation

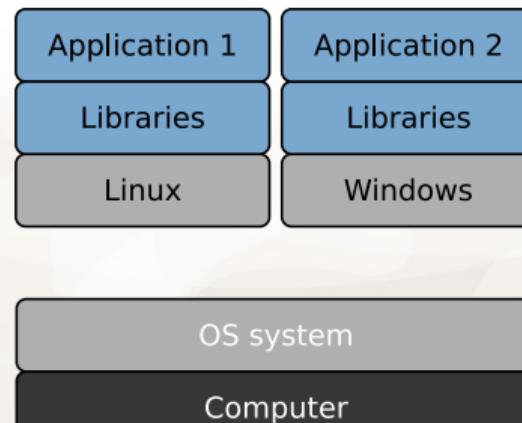
- Start with a computer and a specific OS
- Inside, we installed a new  application
-  need some dependencies
- We tested the last  version -> might be conflicts



Example of R and package installation

hardware virtualisation

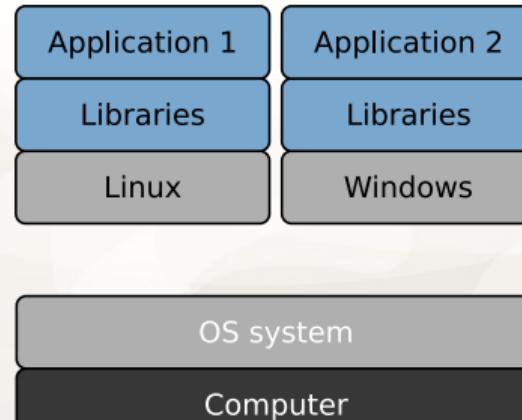
- If we want a software from a different OS ?



Example of R and package installation

hardware virtualisation

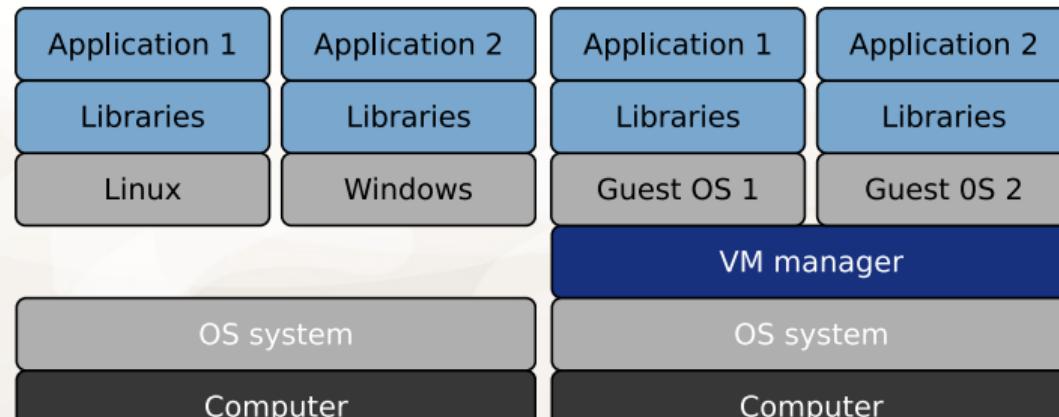
- If we want a software from a different OS ?
- A dual boot ?



Example of R and package installation

hardware virtualisation

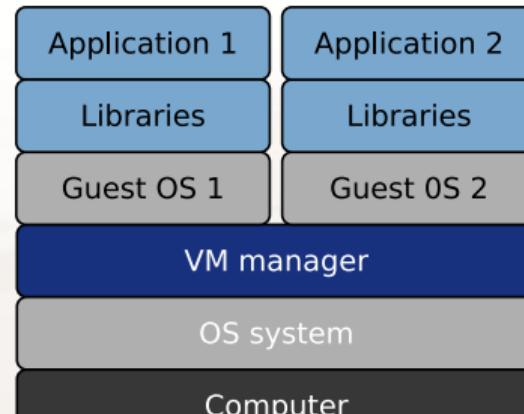
- If we want a software from a different OS ?
- A dual boot ?
- Use virtual machines



Example of R and package installation

hardware virtualisation

- If we want a software from a different OS ?
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- Each application on a different and independant environment



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- Use virtual machines
- Each application on a different and independant environment
- Virtual machine could be transferred to another computer
- Redundancy between VMs
- Heavy to set up
- No automation

Oracle VM VirtualBox Manager

Tools

New Settings Discard Show ▾

ovs34-efi Powered Off	General Name: ubuntu-18.04 Operating System: Ubuntu (64-bit) Settings File Location: /Users/scr/VirtualBox/ubuntu-18.04	Preview
ubuntu-18.04 Running	System Base Memory: 4096 MB Boot Order: Optical, Hard Disk Acceleration: VT-x/AMD-V, Nested Paging, KVM Paravirtualization	Preview
win2016srv Running	General Name: win2016srv Operating System: Windows 2016 (64-bit) Settings File Location: /Users/scr/VirtualBox/win2016srv	Preview
centos7 Powered Off	System Base Memory: 8192 MB Boot Order: Hard Disk, Optical, Floppy Acceleration: VT-x/AMD-V, Nested Paging, PAE/NX	Preview
OracleLinux7 Running	General Name: OracleLinux7 Operating System: Oracle (64-bit) Settings File Location: /Users/scr/VirtualBox/OracleLinux7	Preview
OracleLinux6 Powered Off	System Base Memory: 8192 MB Processors: 2 Boot Order: Hard Disk, Optical Acceleration: VT-x/AMD-V, Nested Paging, PAE/NX, KVM Paravirtualization	Preview
ol7-vbox6 Powered Off		

Example of R and package installation

Containers

- "Trick" applications into believing that they are in a different OS than the host's

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- Named containers :

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- Named containers :
- Avoid redundancy

OS system

Computer

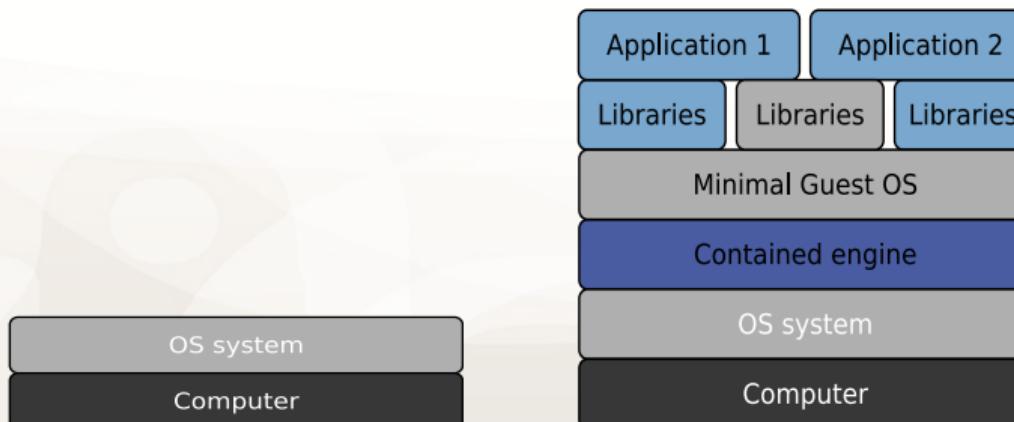
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- Named containers :
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Example of R and package installation

Containers

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- Named containers :
- Avoid redundancy
- Speed
 - Faster installation
 - No boot time

Example of R and package installation

Containers

- "Trick" applications into believing that they are in a different OS than the host's



- Named containers :
- Avoid redundancy
- Speed
 - Faster installation
 - No boot time
- Lightweight
 - Minimal base OS
 - Minimal set of library and global environment
 - Easy sharing of application



rstudio

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Trusted Content

 Docker Official Image ⓘ Verified Publisher ⓘ Sponsored OSS ⓘ

Operating Systems

 Linux Windows

Architectures

 ARM ARM 64 IBM POWER IBM Z PowerPC 64 LE

1 - 25 of 2 061 results for rstudio.

Best Match



ibmcom/rstudio-ppc64le

VERIFIED PUBLISHER

By IBM • Updated 3 years ago

Integrated development environment (IDE) for R

Linux ppc64le

487 4

Downloads Stars



wholelake/rstudio-base

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By wholelake • Updated 4 years ago

Linux x86-64

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By bioconductor • Updated 16 days ago

Linux x86-64

23 0

Downloads Stars



truecharts/rstudio

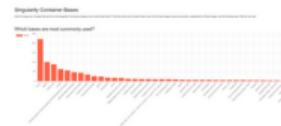
SPONSORED OSS

By truecharts • Updated 11 days ago

Linux x86-64

5 0

Downloads Stars



All repos 1334

rstudio

Stack	Description	Singularity* recipe	Topics	QC	Stars	Watchers
grst/rstudio-server-conda	Run Rstudio Server in a conda environment	0		license MIT last commit October 2021	106	3
nickjer/singularity-rstudio	RStudio Server in a Singularity container	0.1	rstudio-server, singularity-image	license MIT last commit June 2021	40	5
singularityhub/singularity-compose-examples	A simple example of running a MongoDB instance to query a database	0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	singularity-compose, mongodb	license not specified last commit August	12	5
OSC/bc_osc_rstudio_server	Batch Connect - OSC RStudio Server	0		license MIT last commit June	6	10
RBigData/singularity	Singularity configurations for R and pbdr packages.	0 1 2 3 4 5 6 7 8		license BSD-2-Clause last commit October 2019	3	4

- Docker is not easy to use on a cluster system
- Docker private company choices

Example of R and package installation

Conda use

- Separate each application in its own environment **CONDA**

Conda env

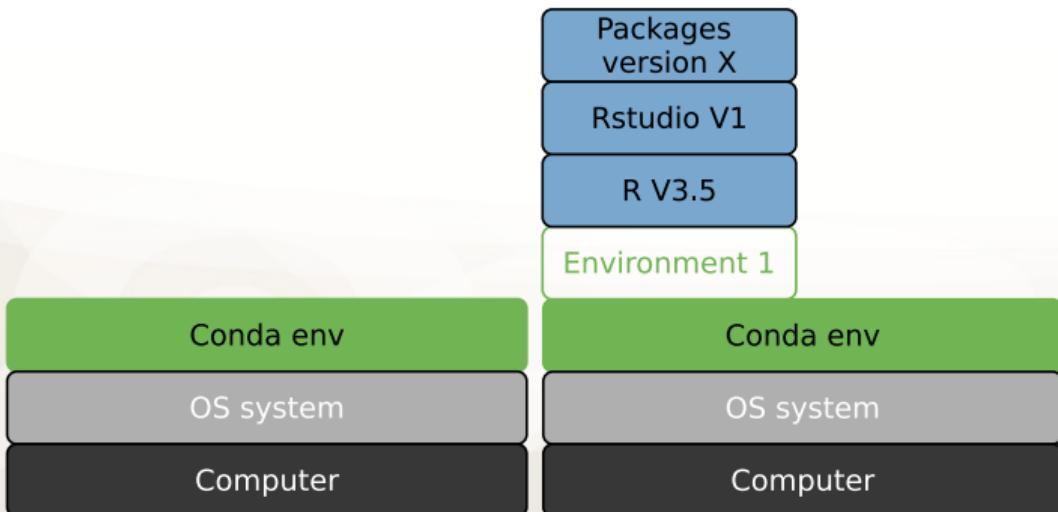
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Example of R and package installation

Conda use

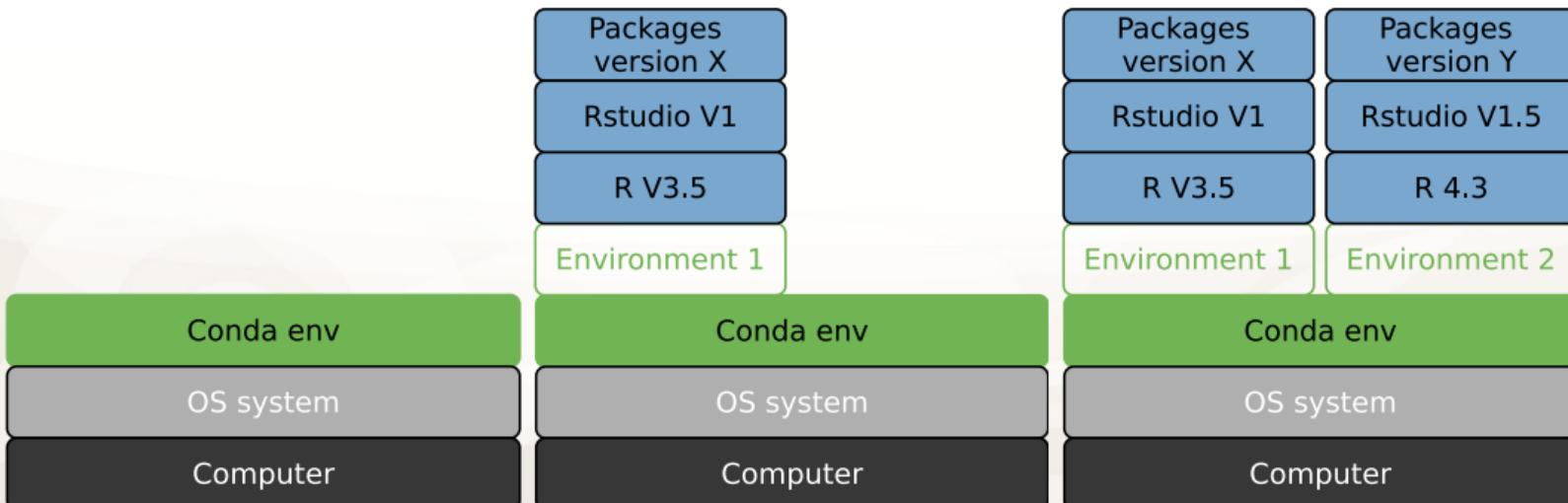
- Separate each application in its own environment **CONDA**
- A tool version = a conda environment



Example of R and package installation

Conda use

- Separate each application in its own environment **CONDA**
- A tool version = a conda environment
- Create a new environment for a new tool version, an analysis...



Conda system

■ Anaconda

- Open source distribution
- Cross platform
- Available on cluster without admin whrite
- Thousands of available tool in informatic and bioinformatic

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- Same advantages ad Anaconda

Conda system

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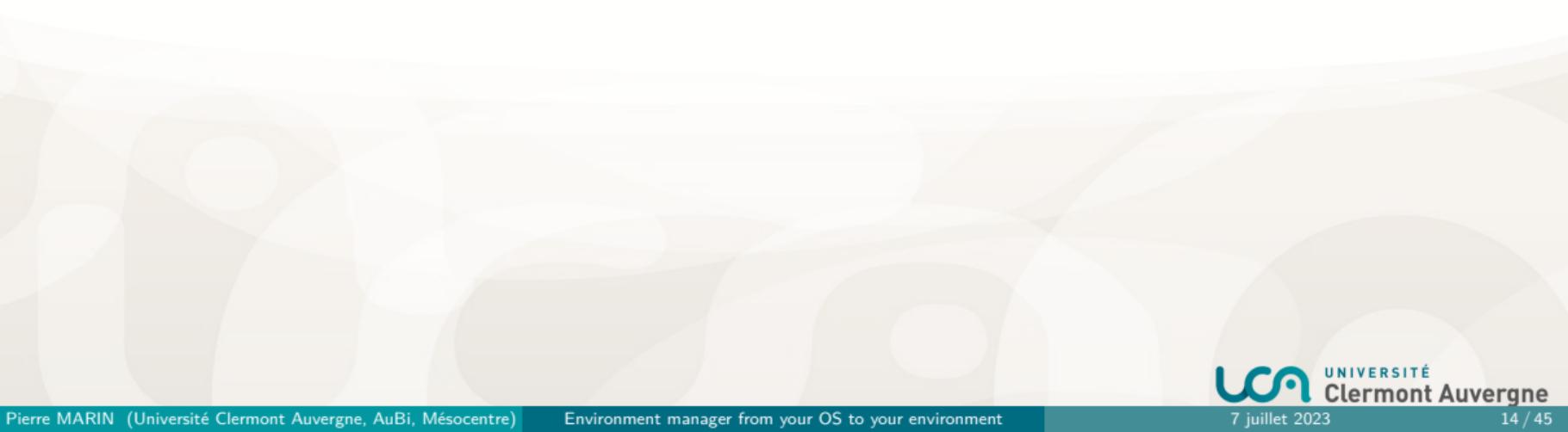
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■ Conda **CONDA**

Conda system



Conda system

CONDA CHEATSHEET	
QUICK START	
Tip: It is recommended to create a new environment for any new project or workflow.	
verify conda install and check version	<code>conda info</code>
update conda in base environment	<code>conda update -n base conda</code>
install latest anaconda distribution (see release notes)	<code>conda install anaconda=2022.08</code>
create a new environment (tip: name environment descriptively)	<code>conda create --name ENVNAME</code>
activate environment (do this before installing packages)	<code>conda activate ENVNAME</code>
CHANNELS AND PACKAGES	
Tip: Package dependencies and platform specifics are automatically resolved when using conda.	
install packages from specified channel	<code>conda install -c CHANNELNAME PKG1 PKG2</code>
list installed packages	<code>conda list</code>
uninstall package	<code>conda uninstall PKGNAME</code>
update all packages	<code>conda update --all</code>
install specific version of package	<code>conda install PKGNAME=3.1.4</code>
install a package from specific channel	<code>conda install CHANNELNAME::PKGNAME</code>
install package with AND logic	<code>conda install "PKGNAME>2.5,<3.2"</code>
install package with OR logic	<code>conda install "PKGNAME [version='2.5 3.2']"</code>
list installed packages with source info	<code>conda list --show-channel-urls</code>
view channel sources	<code>conda config --show-sources</code>
add channel	<code>conda config --add channels CHANNELNAME</code>
set default channel for pkg fetching (targets first channel in channel sources)	<code>conda config --set channel_priority strict</code>
WORKING WITH CONDA ENVIRONMENTS	
Tip: List environments at the beginning of your session. Environments with an asterisk are active.	
Environment manager from your OS to your environment	

The channels and the tools

The tools are packaged and available on several **channels**

. Bioconda : sustainable and comprehensive software distribution for the life sciences *Grüning et al.*, Nature methods, 2018. DOI 10.1038/s41592-018-0046-7



The channels and the tools

The tools are packaged and available on several **channels**

- Conda-forge
- Anaconda
- R
- Bioconda -> Most of the bioinformatic tools

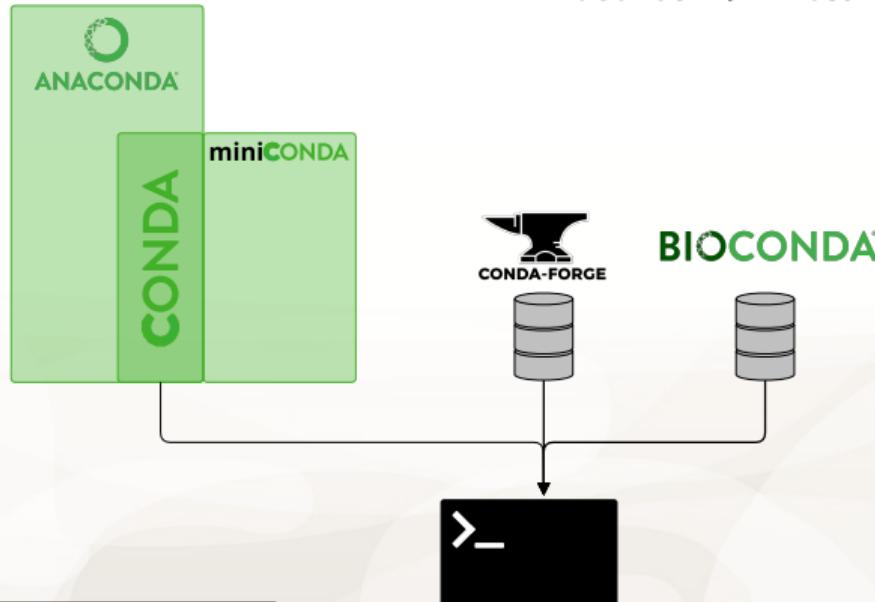
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Basic commands

Create environment

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Search tools

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$ conda search bowtie2  
$ conda search -c bioconda bowtie2
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Basic commands

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$ conda install -c bioconda bowtie2=2.4.5
```

Remove tools

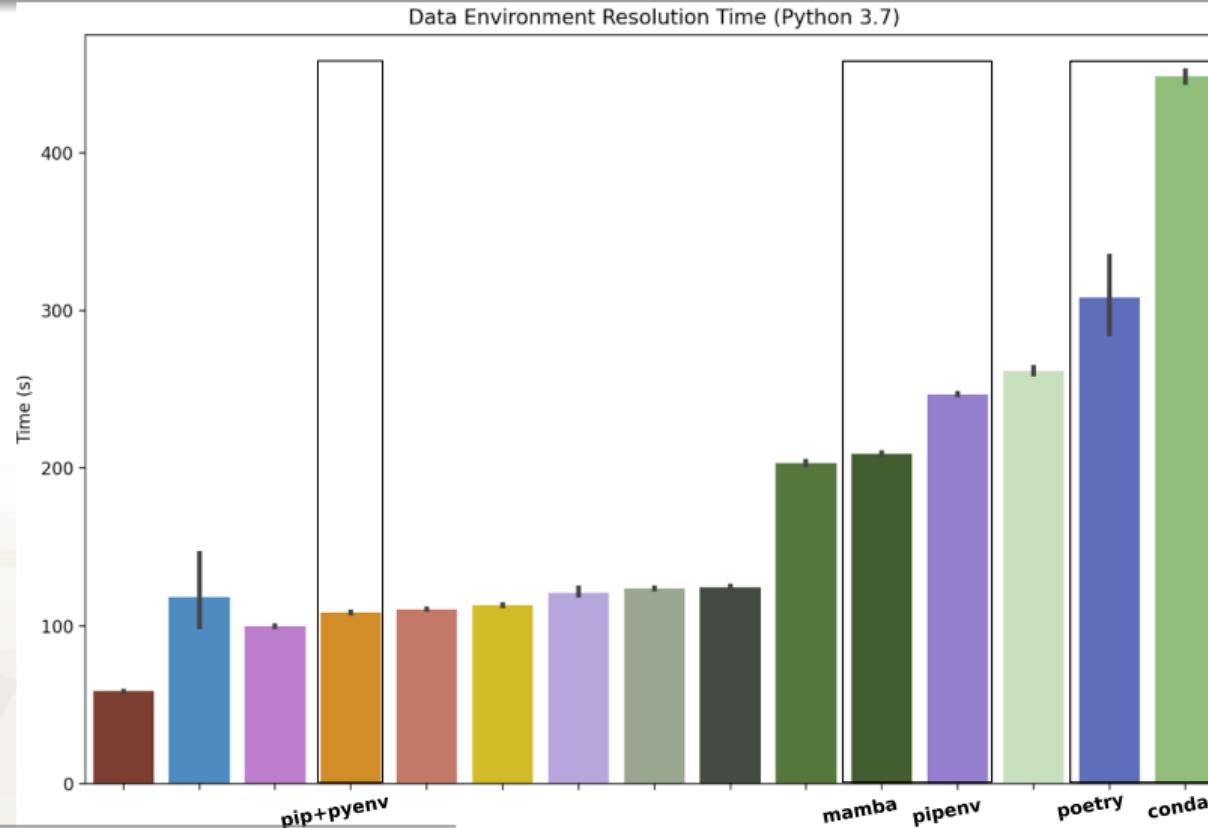
```
$ conda remove bowtie2
```

Environment resolution

Conda also manage environments to keep compatible

- Long time to solve environment resolution
- Can fail and doesn't install

Environment resolution



Modified from <https://www.recursion.com/news/how-recursion-invests-in-developer-experience>

Container technology is not very old

The most famous : 

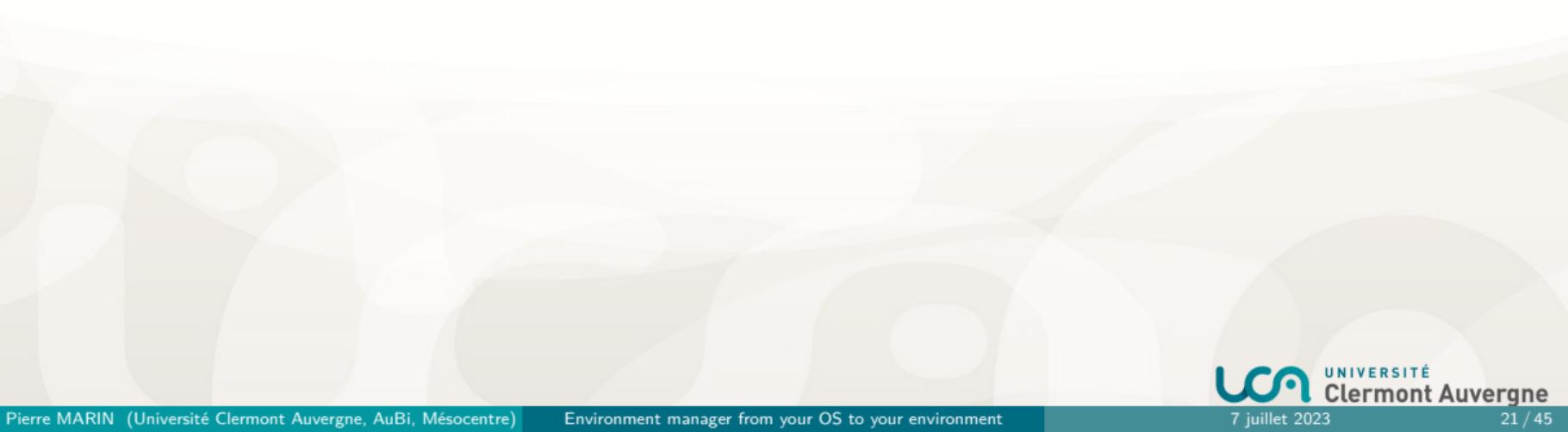
Solomon Hykes was inspired by container port in the world travel



Docker is an open source project, a community and a private company

- Born in 2010
- First public release in 2013
- V 1.0 in 2014
- Open source and free
- Packaged to Ubuntu in 2014 (V14.04)

Term definitions



- Docker image -> "snapshot" immutable file

- Set of libraries, functions
- Static state
- Online Store or share
- Automatically build

- Docker image → "snapshot" immutable file

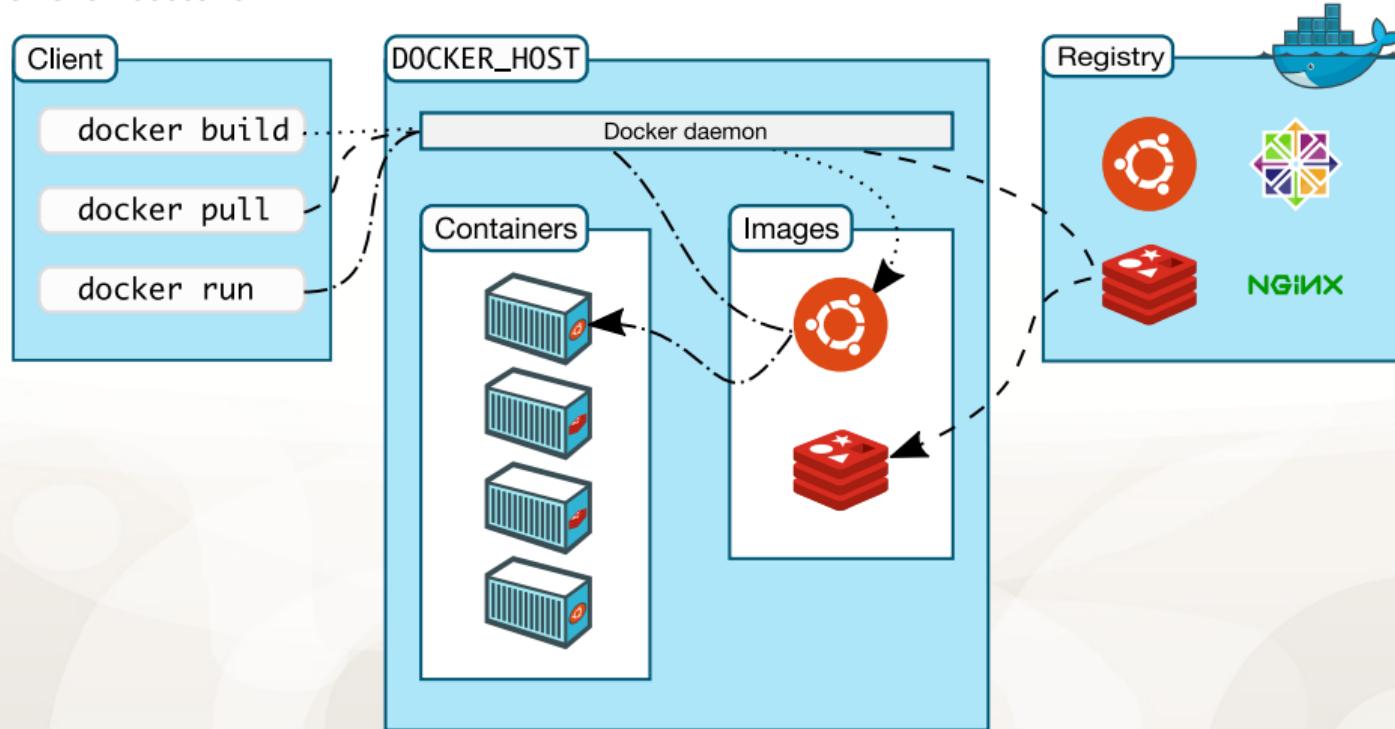
- Set of libraries, functions
 - Static state
 - Online Store or share
 - Automatically build

- Docker container → instance of an image

- Result of the image activation
 - Can be modified
 - Can be turned into an image
 - 1 image → multiple containers

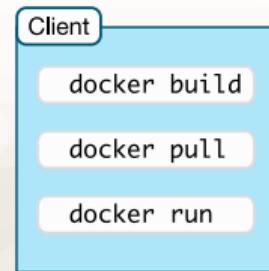
Docker architecture

client-server architecture



Docker client

1 Client to interact with Docker

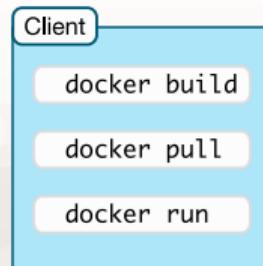


Docker client

- 1 Client to interact with Docker
- 2 Client talk to the daemons (Docker background programs)

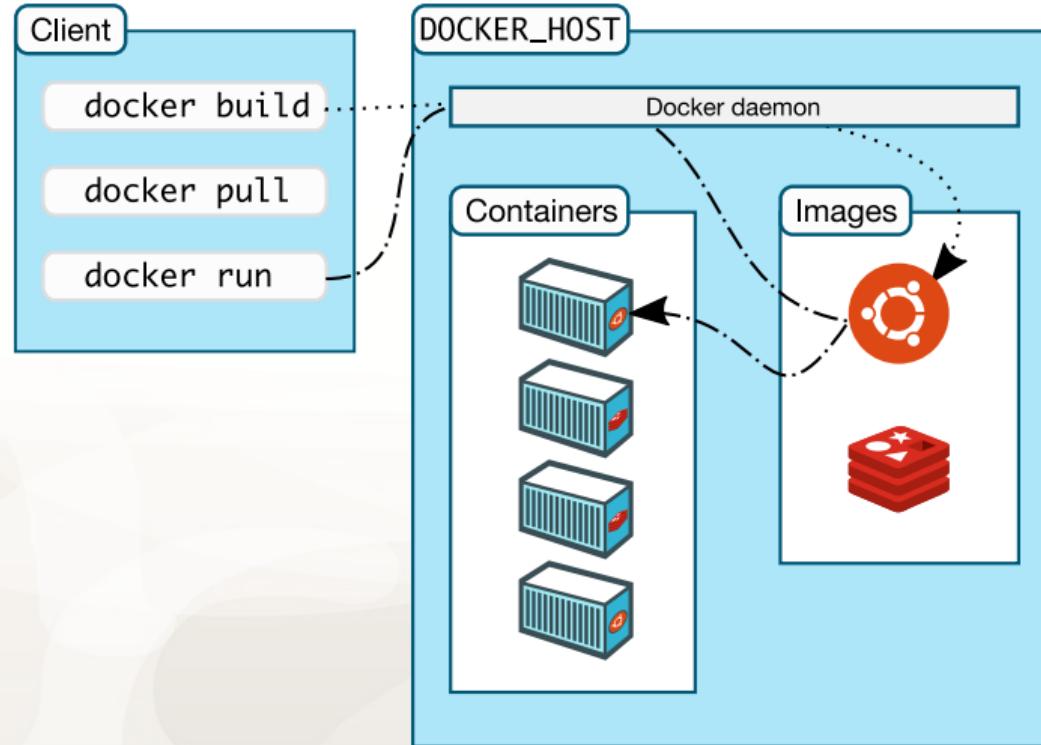
Client

```
$ docker build [path] [url]  
docker build https://github.com/docker/rootfs.git#container:docker  
$ docker pull [image_name]  
docker pull biocontainers/samtools  
$ docker run [image_name]  
docker run biocontainers/samtools
```



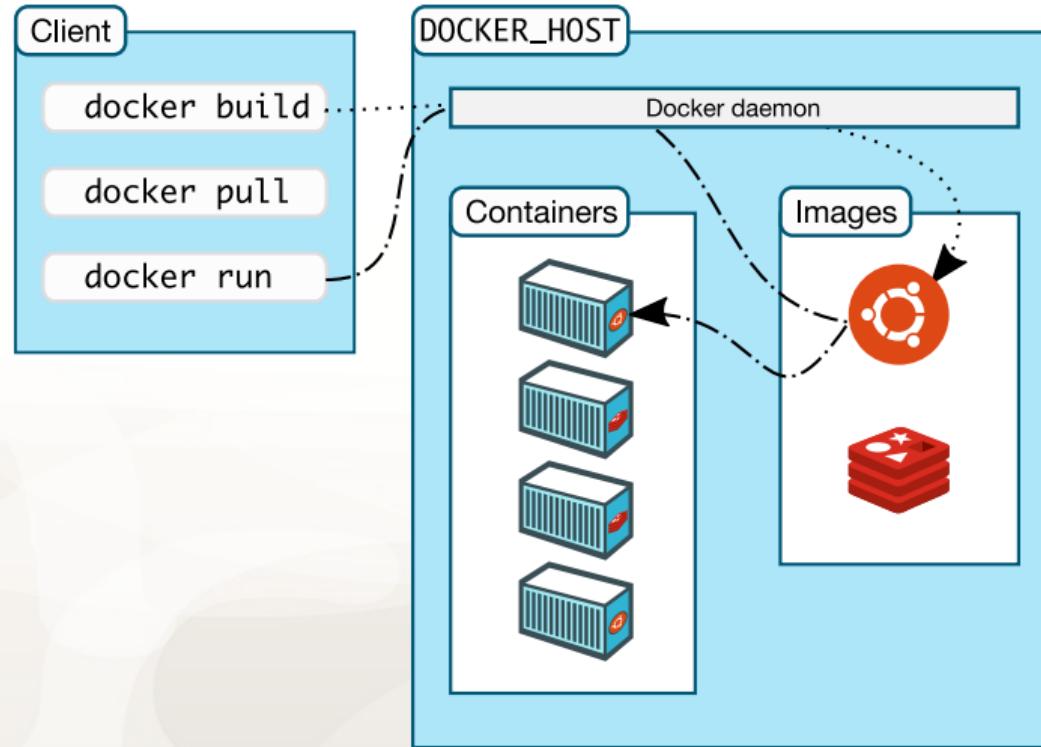
Docker daemon

- 1 Listen client requests



Docker daemon

- 1 Listen client requests
- 2 Manage Docker's images, containers...



Docker registries

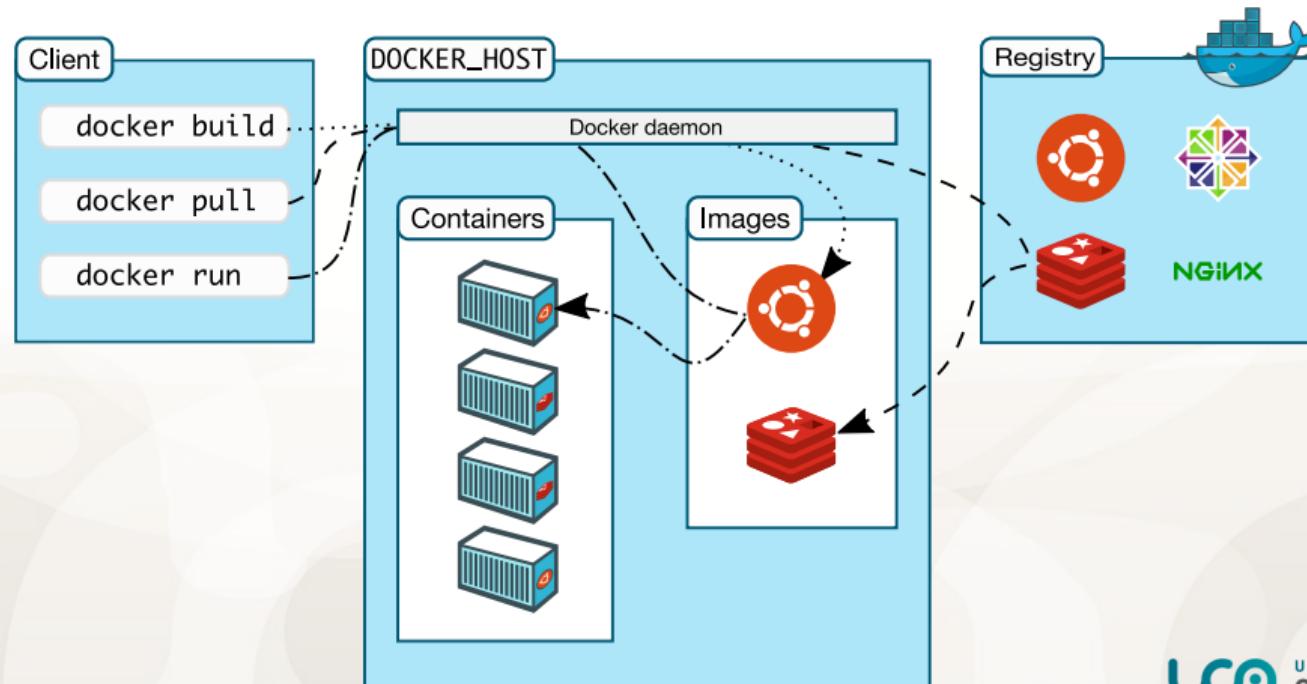
1 Store Docker images

The screenshot shows the Docker Hub search interface. The search bar at the top contains the query 'rstudio'. Below the search bar, there are navigation links for 'Explore', 'Pricing', 'Sign In', and 'Register'. On the left, a sidebar provides filtering options: 'Images', 'Extensions', 'Plugins', 'Docker Official Image', 'Verified Publisher', 'Sponsored OSS', 'Linux', 'Windows', 'ARM', 'ARM 64', 'IBM POWER', 'IBM Z', and 'PowerPC 64 LE'. The main content area displays search results for 'rstudio' with 1 - 25 of 2,061 results. The results are listed in descending order of popularity ('Best Match'). Each result card includes the repository name, publisher information (verified or sponsored), last update, operating system, architecture, and download and star counts.

Repository	Publisher	Last Updated	OS	Architectures	Downloads	Stars
ibmcom/rstudio-ppc64le	IBM	3 years ago	Linux	ppc64le	487	4
wholetale/rstudio-base	wholetale	4 years ago	Linux	x86-64	127	0
bioconductor/rstudio_yescods	bioconductor	16 days ago	Linux	x86-64	23	0
truecharts/rstudio	truecharts	11 days ago	Linux	x86-64	5	0

Docker registries

- 1 Store Docker images
- 2 Docker hub is a public registry



Docker registries

- 1 Store Docker images
- 2 Docker hub is a public registry
- 3 You can run your own registry

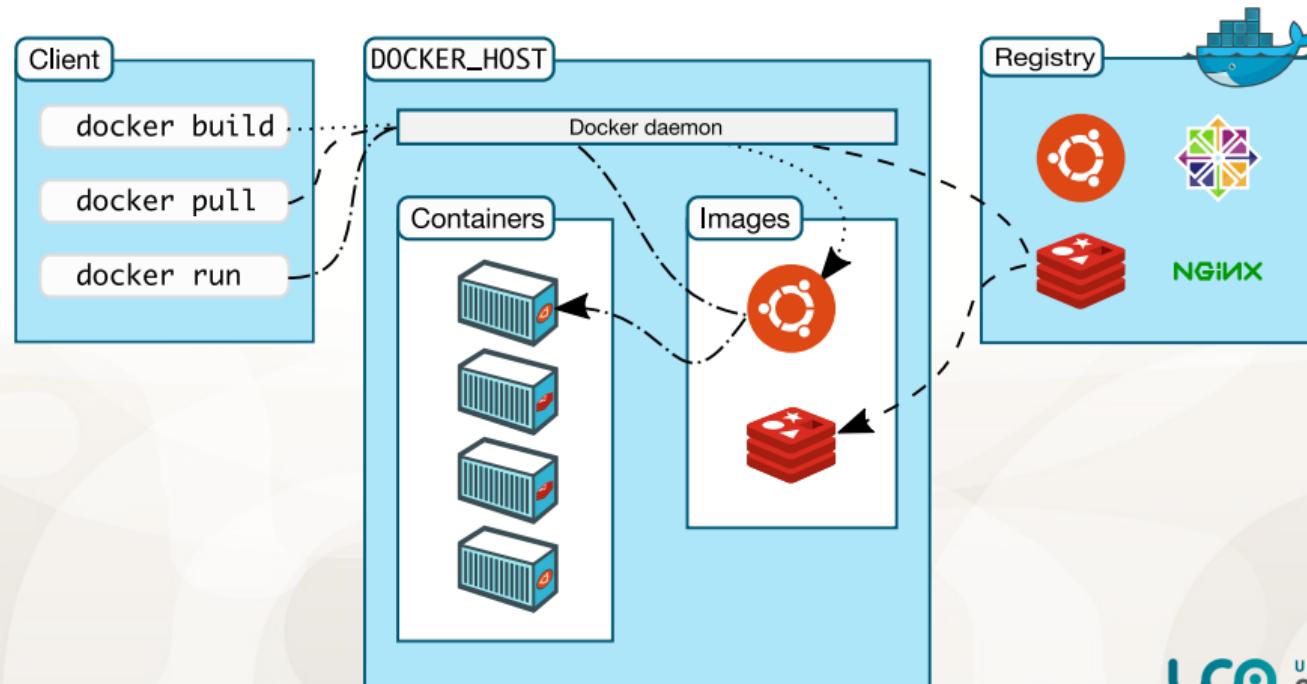


Image layers

Focus on image building

- Layers building

Image layers

Focus on image building

- Layers building
- Several layers to one image

Image layers

Focus on image building

- Layers building
- Several layers to one image
- Some layers shared by images when pulling
- Lighten the download and use of image on your computer

```
$ docker pull debian
Using default tag: latest
latest: Pulling from library/debian
fdd5d7827f33: Pull complete
a3ed95caeb02: Pull complete
Digest: sha256:e7d38b3517548a1c71e41bffe9c8ae6d6d29546ce46bf62159837aad072c90aa
Status: Downloaded newer image for debian:latest
```

Pull me Hello world !

- Try and pull your first image from docker hub

```
$ docker pull [path/url/docker_name]
```

```
$ docker pull hello-world
```

```
Using default tag: latest
```

```
latest: Pulling from library/hello-world
```

```
2db29710123e: Already exists
```

```
Digest: sha256:63421b18c1443a9a85139225293fae7541fb40b7832d9deff80b6a9a75ce3604
```

```
Status: Downloaded newer image for hello-world:latest
```

```
docker.io/library/hello-world:latest
```

Pull me Hello world !

- Now run the hello-world image

```
$ docker image ls
```

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
hello-world	latest	feb5d9fea6a5	17 months ago	13.3kB
assembly_conda	latest	5ea57e9c4563	4 hours ago	2.99GB
assembly_raw	latest	dffe598c3a14	4 hours ago	990MB
condaforge/mambaforge	latest	8562647c2abf	12 days ago	393MB
ubuntu	bionic	b89fba62bc15	2 weeks ago	63.1MB

Pull me Hello world !

■ Now run the hello-world image

```
$ docker run[image_name/image_tag]  
$ docker run hello-world  
Hello from Docker!
```

This message shows that your installation appears to be working correctly.

To generate this message, Docker took the following steps:

1. The Docker client contacted the Docker daemon.
2. The Docker daemon pulled the "hello-world" image from the Docker Hub.
(amd64)
3. The Docker daemon created a new container from that image which runs the executable that produces the output you are currently reading.
4. The Docker daemon streamed that output to the Docker client, which sent it to your terminal.

Build my own image

The basic recipe of Dockerfile

- **FROM** A basic framework (image) as a linux, microsoft for ex.
- **RUN** A command to install a tool

Build my own image

Some few docker specific commands AJOUTER UN LIEN DOCKER POUR LE SITTTTTTEEEE

Instruction	Description
FROM	Image parente
MAINTAINER	Auteur
ARG	Variables passées comme paramètres à la construction de l'image
ENV	Variable d'environnement
LABEL	Ajout de métadonnées
VOLUME	Crée un point de montage
RUN	Commande(s) utilisée(s) pour construire l'image
ADD	(Ajoute un fichier dans l'image *ADD vs COPY)
COPY	Ajoute un fichier dans l'image
WORKDIR	Permet de changer le chemin courant
EXPOSE	Port(s) écouté(s) par le conteneur
USER	Nom d'utilisateur ou UID à utiliser
ONBUILD	Instructions exécutées lors de la construction d'images enfants
CMD	Exécuter une commande au démarrage du conteneur

Build my own image

Dockerfile skeleton

The basic recipe of Dockerfile

- **FROM** A basic framework (image) as a linux, microsoft for ex.
- **RUN** A command to install a tool

```
FROM ubuntu:bionic
ARG USER="Coco"
LABEL maintainer.email="coco@lasticot.fr"
RUN apt-get update
RUN echo "HELLO WORLD !"
```

Build command

AJOUTER UN SOUS TITRE POUR EXPLICITE RLE CAS DE GITHUB

AJOUTER code gras pour les commandes

\$ docker build [url/path] --tag [docker_name]

special case with github url like :

[url]\#[branch_name] [file_path]

**\$ docker build https://github.com/mesocentre-clermont-auvergne/formation_fair.git **
\#main:/fair_encapsulation/fair_encapsulation_TP/fair_encapsulation_containers/fair_e
-t assembly_raw

Export docker image

```
$ docker save [image_name/ID] > [image_name].tar
```

Docker Cheat Sheet



Build

Build an image from the Dockerfile in the current directory and tag the image

```
docker build -t myimage:1.0 .
```

List all images that are locally stored with the Docker Engine

```
docker image ls
```

Delete an image from the local image store

```
docker image rm alpine:3.4
```



Share

Pull an image from a registry

```
docker pull myimage:1.0
```

Retag a local image with a new image name and tag

```
docker tag myimage:1.0 myrepo/myimage:2.0
```

Push an image to a registry

```
docker push myrepo/myimage:2.0
```



Run

Run a container from the Alpine version 3.9 image, name the running container "web" and expose port 5000 externally, mapped to port 80 inside the container.

```
docker container run --name web -p 5000:80 alpine:3.9
```

Stop a running container through SIGTERM

```
docker container stop web
```

Stop a running container through SIGKILL

List the running containers (add `--all` to include stopped containers)

```
docker container ls
```

Delete all running and stopped containers

```
docker container rm -f $(docker ps -aq)
```

Print the last 100

lines of a container's logs

```
docker container logs --tail 100 web
```



Docker Management

All commands below are called as options to the base `docker` command. Run `docker <command> --help` for more information on a particular command.

<code>app*</code>	<i>Docker Application</i>
<code>assemble*</code>	<i>Framework-aware builds (Docker Enterprise)</i>
<code>builder</code>	<i>Manage builds</i>
<code>cluster</code>	<i>Manage Docker clusters (Docker Enterprise)</i>
<code>config</code>	<i>Manage Docker configs</i>
<code>context</code>	<i>Manage contexts</i>
<code>engine</code>	<i>Manage the docker Engine</i>
<code>image</code>	<i>Manage images</i>
<code>network</code>	<i>Manage networks</i>
<code>node</code>	<i>Manage Swarm nodes</i>
<code>plugin</code>	<i>Manage plugins</i>
<code>registry*</code>	<i>Manage Docker registries</i>
<code>secret</code>	<i>Manage Docker secrets</i>
<code>service</code>	<i>Manage services</i>
<code>stack</code>	<i>Manage Docker stacks</i>
<code>swarm</code>	<i>Manage swarm</i>
<code>system</code>	<i>Manage Docker</i>

DOCKER COMPOSE CHEAT SHEET

File

structure

```
services:
  container1:
    properties: values

  container2:
    properties: values
```

```
networks:
  network:
```

```
volumes:
  volume:
```

Types

value

```
key: value
```

array

```
key:
  - value
  - value
```

dictionary

```
master:
  key: value
  key: value
```

Properties

build

```
build image from dockerfile
in specified directory
```

container:

```
  build: ./path
  image: image-name
```

image

```
use specified image
```

```
image: image-name
```

container_name

```
define container name to access
it later
```

```
container_name: name
```

volumes

```
define container volumes to
persist data
```

volumes:

```
  - /path:/path
```

command

```
override start command for the
container
```

```
command: execute
```

environment

```
define env variables for the
container
```

environment:

```
  KEY: VALUE
  ...
  environment:
    - KEY=VALUE
```

env_file

```
define a env file for the
container to set and override
env variables
```

```
env_file: .env
```

```
  ...
  env_file:
    - .env
```

restart

```
define restart rule
(no, always, on-failure, unless-
stopped)
```

expose:

```
  - "9999"
```

networks

```
define all networks for the
container
```

networks:

```
  - network-name
```

ports

```
define ports to expose to other
containers and host
```

ports:

```
  - "9999:9999"
```

expose

```
define ports to expose only to
other containers
```

expose:

```
  - "9999"
```

network_mode

```
define network driver
(bridge, host, none, etc.)
```

```
network_mode: host
```

depends_on

```
define build, start and stop
order of container
```

depends_on:

```
  - container-name
```

Other

idle container

```
send container to idle state
> container will not stop
```

```
command: tail -f /dev/null
```

named volumes

```
create volumes that can be used in
the volumes property
```

services:

```
  container:
    image: image-name
    volumes:
      - data-
    volume:/path/to/dir
```

volumes:

```
  data-volume:
```

networks

```
create networks that can be used
in the networks property
```

networks:

```
  frontend:
    driver: bridge
```



Singularity history

- Also a container manager as Docker



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- Open-source project

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- Release in 2015
- Fork project in 2020 with now AppTainer (linux foundation) and SingularityCE
- HPC compatible, no root write, integrate ressource managers (slurm)
- Could use Docker images

Singularity commands

Docker command

```
$ docker search [image_name]  
$ docker pull [image_name]  
$ docker run [image_name]
```

Singularity commands

Docker command

```
$ docker search [image_name]  
$ docker pull [image_name]  
$ docker run [image_name]
```

Singularity commands

```
$ singularity search [image_name]  
$ singularity pull [image_name]  
$ singularity run [image_name]
```

Singularity and Docker

Singularity can use Docker images

- from docker hub
- from docker file

```
$ singularity build [new_image_name] docker-archive://[image_name].tar
$ singularity run [new_image_name]
$ singularity pull docker://debian:latest
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
Getting image source signatures
Copying blob f606d8928ed3 done
Copying config 0311b76201 done
Writing manifest to image destination
Storing signatures
2022/10/06 10:50:41  info unpack layer: sha256:f606d8928ed378229f2460b94b504cca239fb9
INFO:    Creating SIF file...
```

Singularity recipe

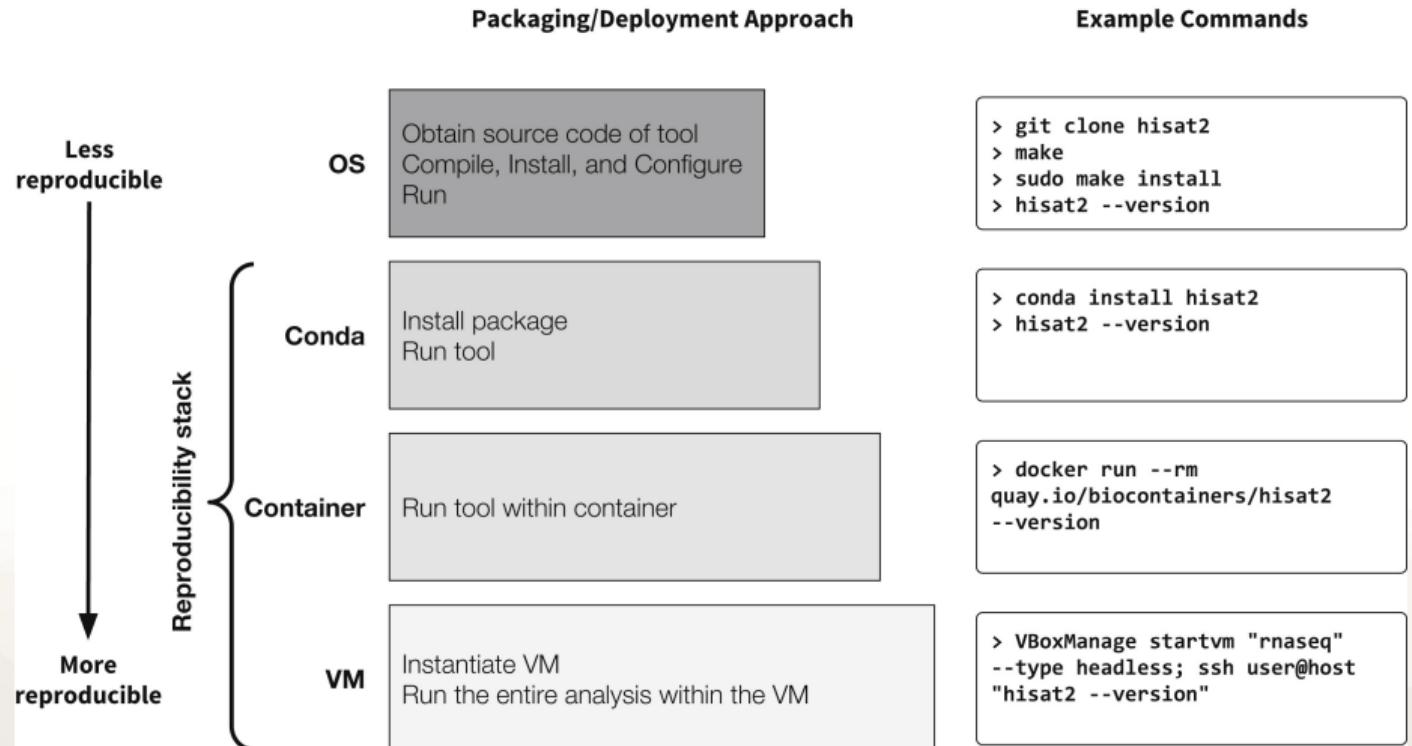
Bootstrap	base you want to use (e.g., docker, debootstrap, shub)
From	named container you want to use
%help	help text to the user
%setup	executed command on the host system outside the container
%files	allow to copy file to the containers
%labels	store metadata with your container,
%environment	environment variables sourced at runtime
%post setup	command of your container
%runscript	started when container is running
%test	command to test the image build

Singularity recipe

Bootstrap: docker

From: ubuntu:bionic

```
%help
Help me. I'm in the container.
%labels
    Maintainer "coco l'asticot"
%environment
    VADER=badguy
    LUKE=goodguy
    export VADER LUKE
%post
    echo "Hello World !"
%runscript
    echo "Rooooar!"
```



1

1. Practical Computational Reproducibility in the Life Sciences Grüning et al, Cell Systems, 2018. DOI 10.1101/j.cels.2018.03.014

Some recommandations

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. Recommendations for the packaging and containerizing of bioinformatics software Gruening, F1000 Research, 2019.
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- Check the license of the software
- Make your package or container discoverable
- Provide reproducible and documented builds
- Provide helpful usage message

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Encapsulation PRACTICE

Conda, Singularity and Docker