

Environment manager from your OS to your environment

Encapsulation levels using Conda, Docker and Singularity



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25 novembre 2022

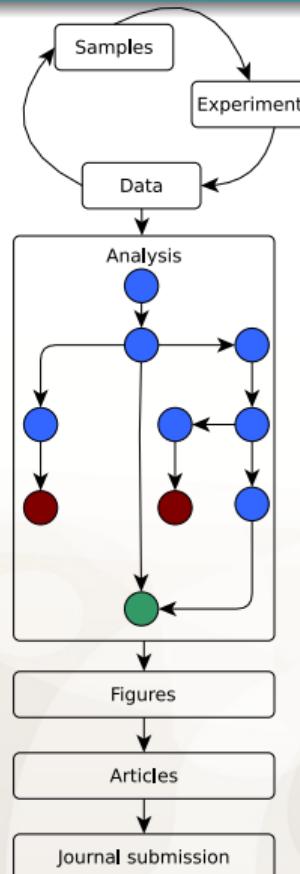


. This work is based on the IFB and I2BC formation offer

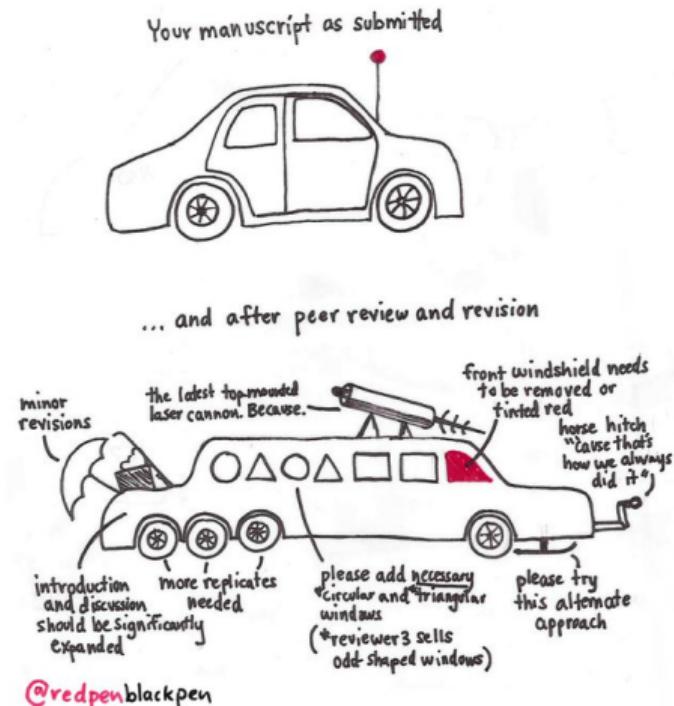
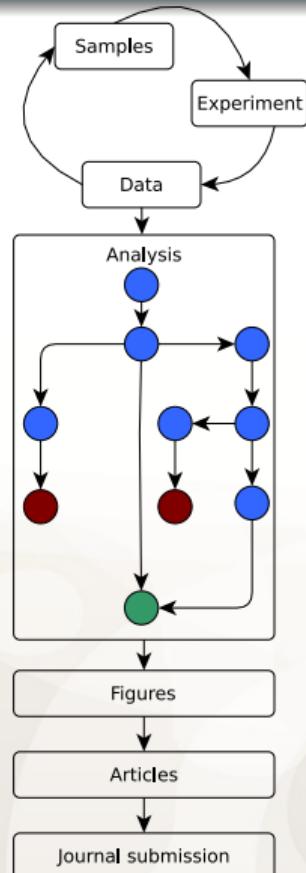
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 - Retry my results
 - The use of packaging
 - Example with R
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 - How conda works
- 3 Manage your hardware configuration
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- 4 Manage your OS configuration
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- 6 A second level, the containers
 - Docker
 - Singularity
- 7 Conclusion about encapsulation
 - Integrative levels of encapsulation
 - Recommandations

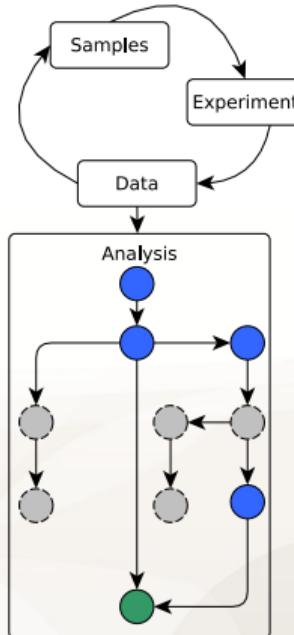
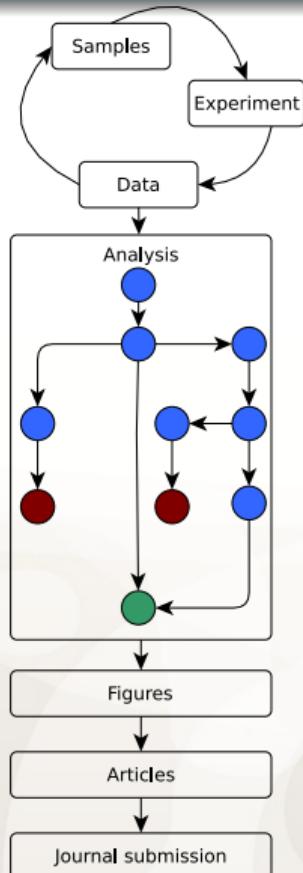
A classic use case



A classic use case



A classic use case



A classic use case

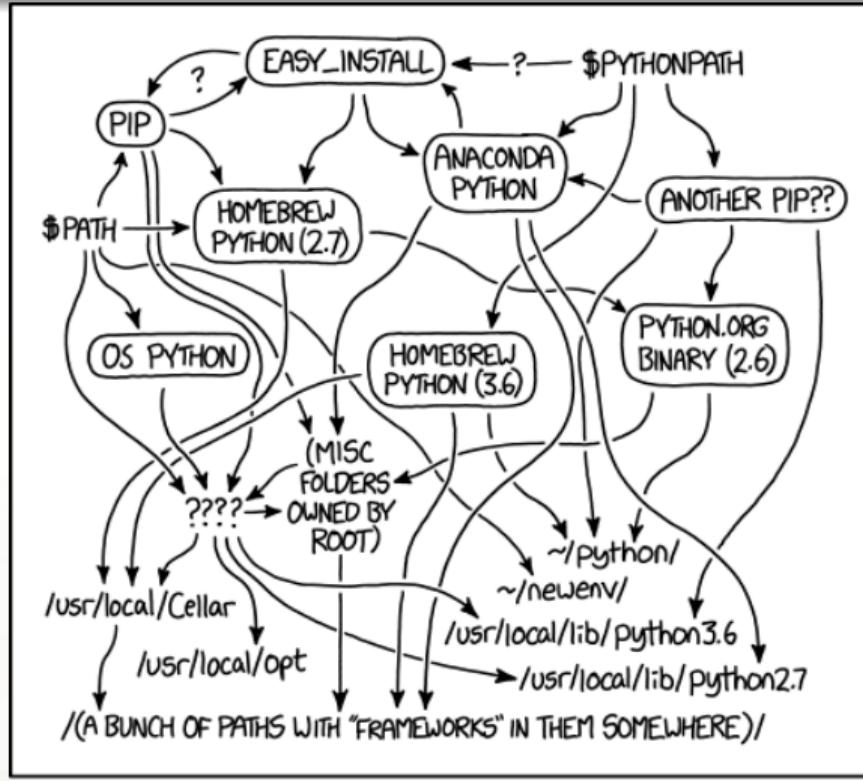
What are the changes ?

- 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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- Hardware virtualisation (virtual machines)

Encapsulation levels

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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

Classical installation

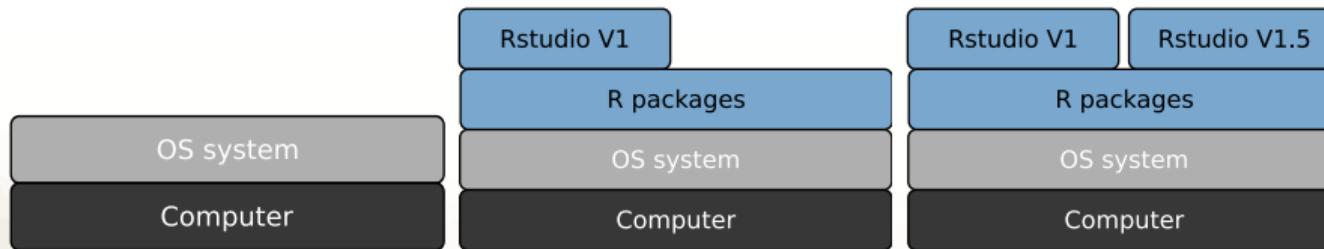
- Start with a computer and a specific OS
- Inside, we installed a new  application



Example of R and package installation

Classical installation

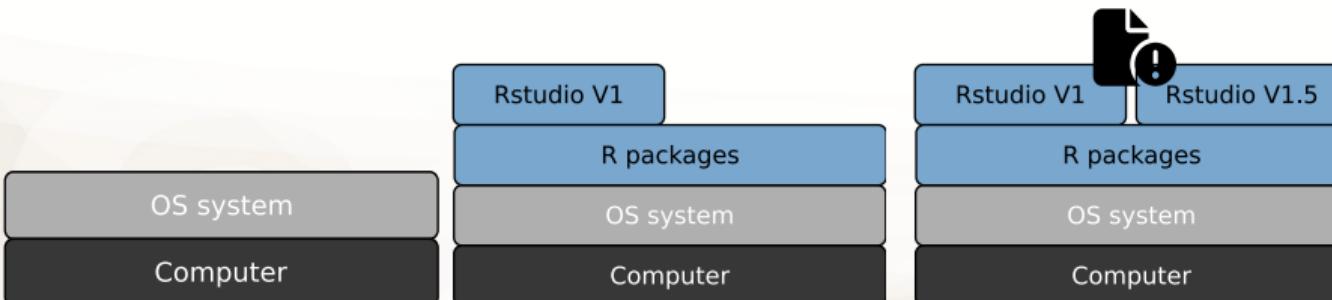
- Start with a computer and a specific OS
- Inside, we installed a new  application
-  need some dependencies



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

Conda use

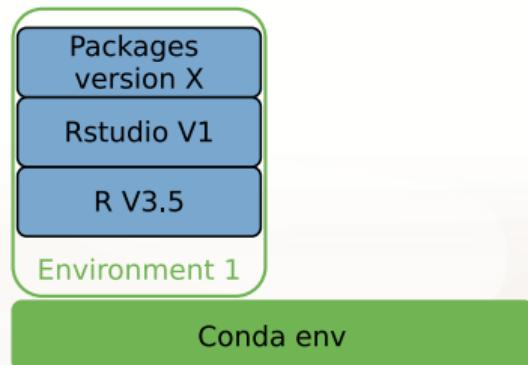
- Separate each application in its own environment **CONDA**

Conda env

Example of R and package installation

Conda use

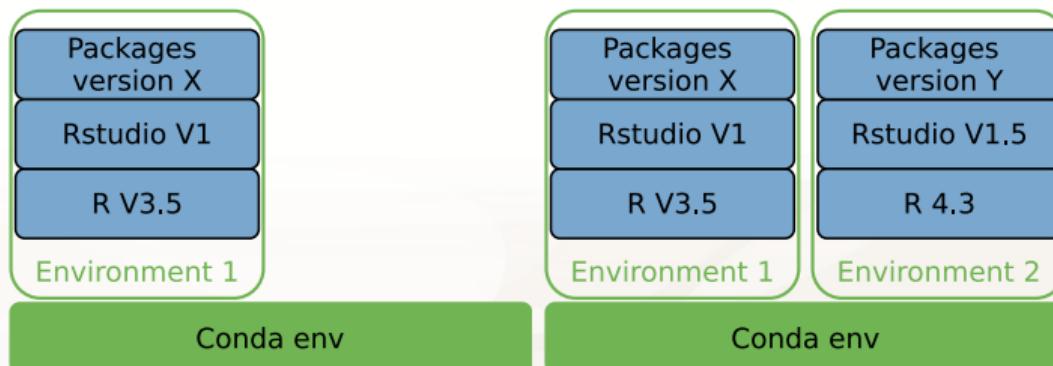
- Separate each application in its own environment **CONDA**
- A tool version = a conda environment



Example of R and package installation

Conda use

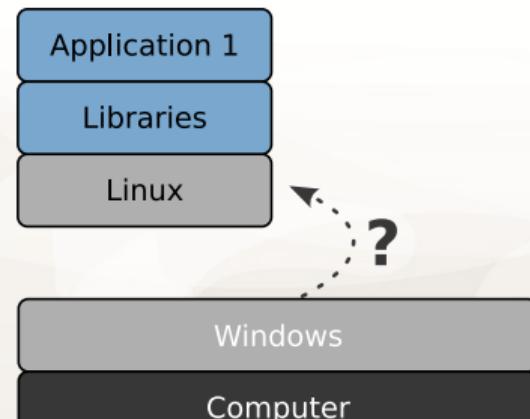
- Separate each application in its own environment **CONDA**
- A tool version = a conda environment
- Create a new environment for a new tool version, an analysis...



Example of R and package installation

hardware virtualisation

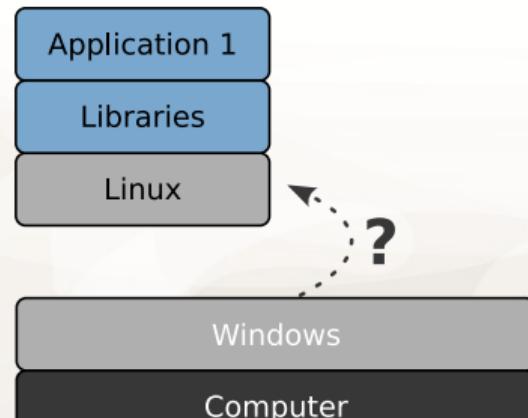
- If we want a software from a different OS ?



Example of R and package installation

hardware virtualisation

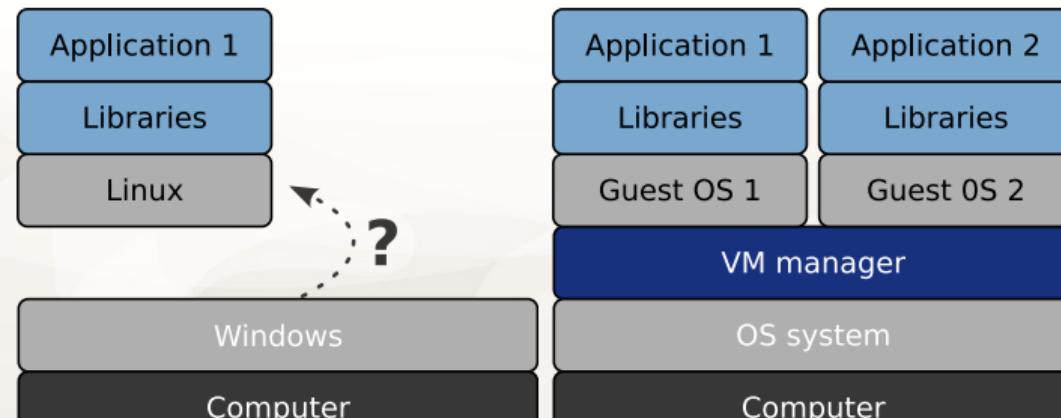
- If we want a software from a different OS ?
- A dual boot ?



Example of R and package installation

hardware virtualisation

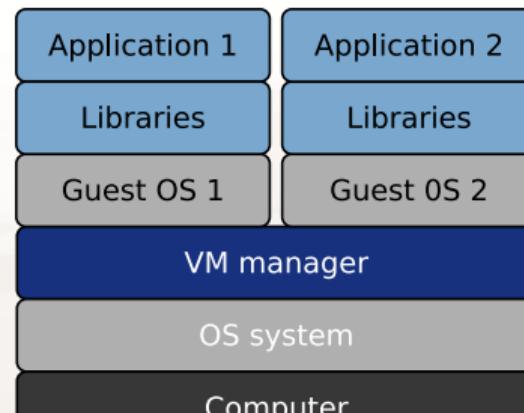
- If we want a software from a different OS ?
- A dual boot ?
- Use virtual machines



Example of R and package installation

hardware virtualisation

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



Example of R and package installation

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- If we want a software from a different OS ?
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- Redundancy between VMs

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hardware virtualisation

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hardware virtualisation

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

Icon	Name	Status
	ovs34-efi	Powered Off
	ubuntu-18.04	Running
	win2016srv	Running
	centos7	Powered Off
	OracleLinux7	Running
	OracleLinux6	Powered Off
	ol7-vbox6	Powered Off

General

Name: ubuntu-18.04
Operating System: Ubuntu (64-bit)
Settings File Location: /Users/scr/VirtualBox/ubuntu-18.04

System

Base Memory: 4096 MB
Boot Order: Optical, Hard Disk
Acceleration: VT-x/AMD-V, Nested Paging, KVM Paravirtualization

Preview

General

Name: win2016srv
Operating System: Windows 2016 (64-bit)
Settings File Location: /Users/scr/VirtualBox/win2016srv

System

Base Memory: 8192 MB
Boot Order: Hard Disk, Optical, Floppy
Acceleration: VT-x/AMD-V, Nested Paging, PAE/NX

Preview

General

Name: OracleLinux7
Operating System: Oracle (64-bit)
Settings File Location: /Users/scr/VirtualBox/OracleLinux7

System

Base Memory: 8192 MB
Processors: 2
Boot Order: Hard Disk, Optical
Acceleration: VT-x/AMD-V, Nested Paging, PAE/NX, KVM Paravirtualization

Preview

Example of R and package installation

Containers

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

Example of R and package installation

Containers

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- Named containers :

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

OS system

Computer

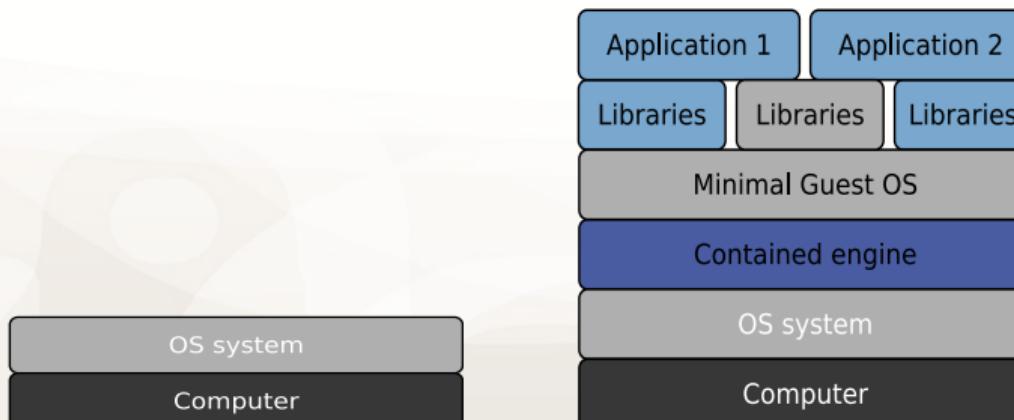
Example of R and package installation

Containers

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



- Named containers :
- Avoid redundancy



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

Filters

Products

 Images Extensions Plugins

Trusted Content

 Docker Official Image ⓘ Verified Publisher ⓘ Sponsored OSS ⓘ

Operating Systems

 Linux Windows

Architectures

 ARM ARM 64 IBM POWER

1 - 25 of 2 123 results for rstudio.

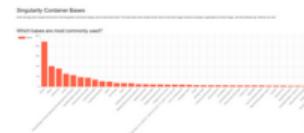
Best Match ▾

**ibmcom/rstudio-ppc64le**  VERIFIED PUBLISHER
By IBM • Updated 3 years ago
Integrated development environment (IDE) for R
Linux ppc64le

**whohetale/rstudio-base**  SPONSORED OSS
By whohetale • Updated 5 years ago
Linux x86-64

**bioconductor/rstudio_yescds**  SPONSORED OSS
By bioconductor • Updated 2 months ago
Linux x86-64

521 4
Downloads Stars167 0
Downloads Stars62 0
Downloads Stars



All repos 1385

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 october	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

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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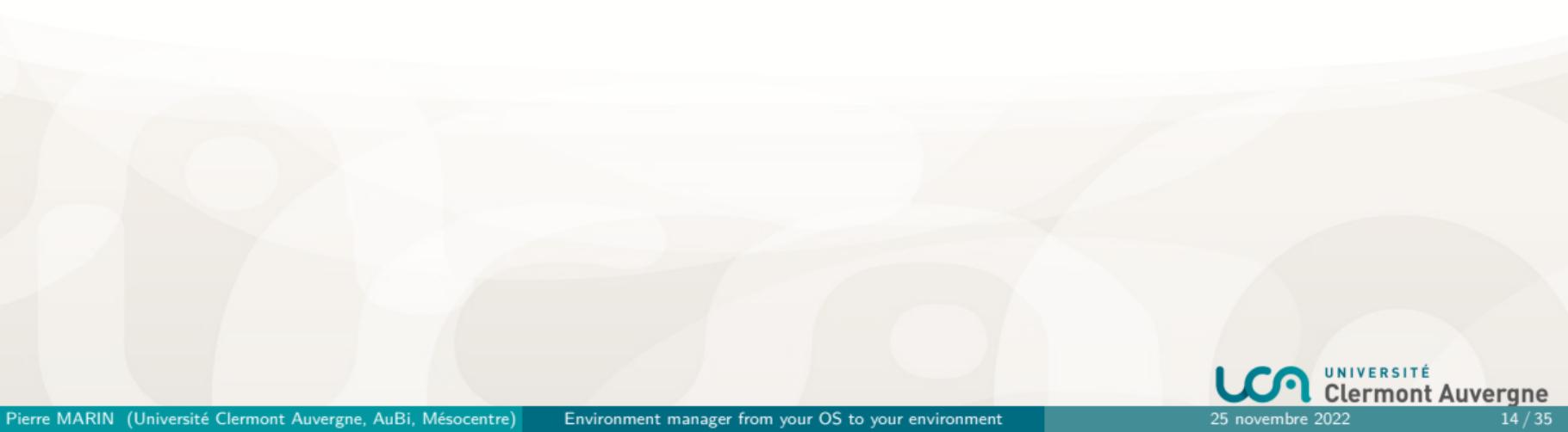
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■ Conda **CONDA**

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

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

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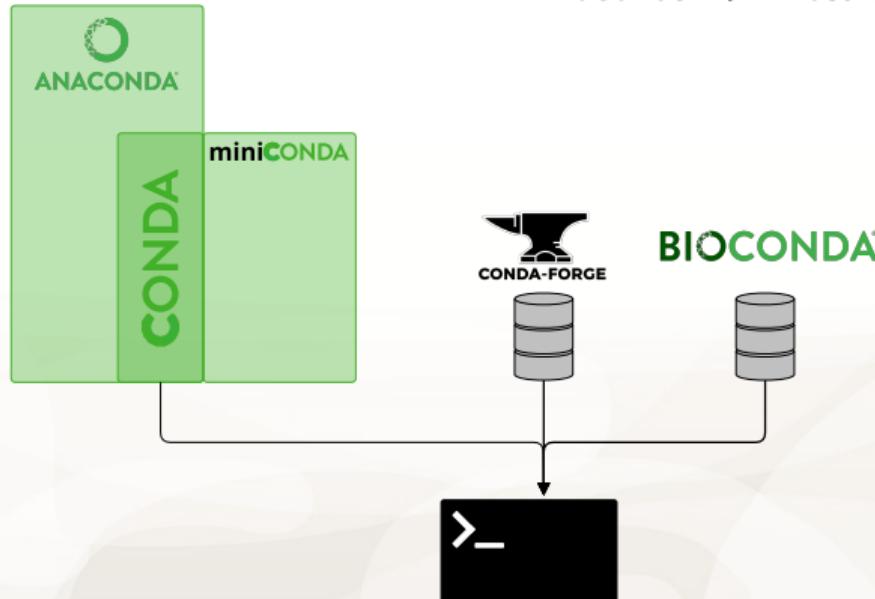
- Conda-forge
- Anaconda
- R
- Bioconda -> Most of the bioinformatic tools

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- Conda-forge
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Basic commands

Create environment

```
$ conda create -n [env_name]  
$ conda activate [env_name]  
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Search tools

```
$ conda search bowtie2  
$ conda search -c bioconda bowtie2
```

Basic commands

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$ conda create -n [env_name]  
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list environment or packages

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$ conda env list  
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Search tools

```
$ conda search bowtie2  
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```

Install tools

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

Basic commands

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```
$ conda install bowtie2  
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```

Remove tools

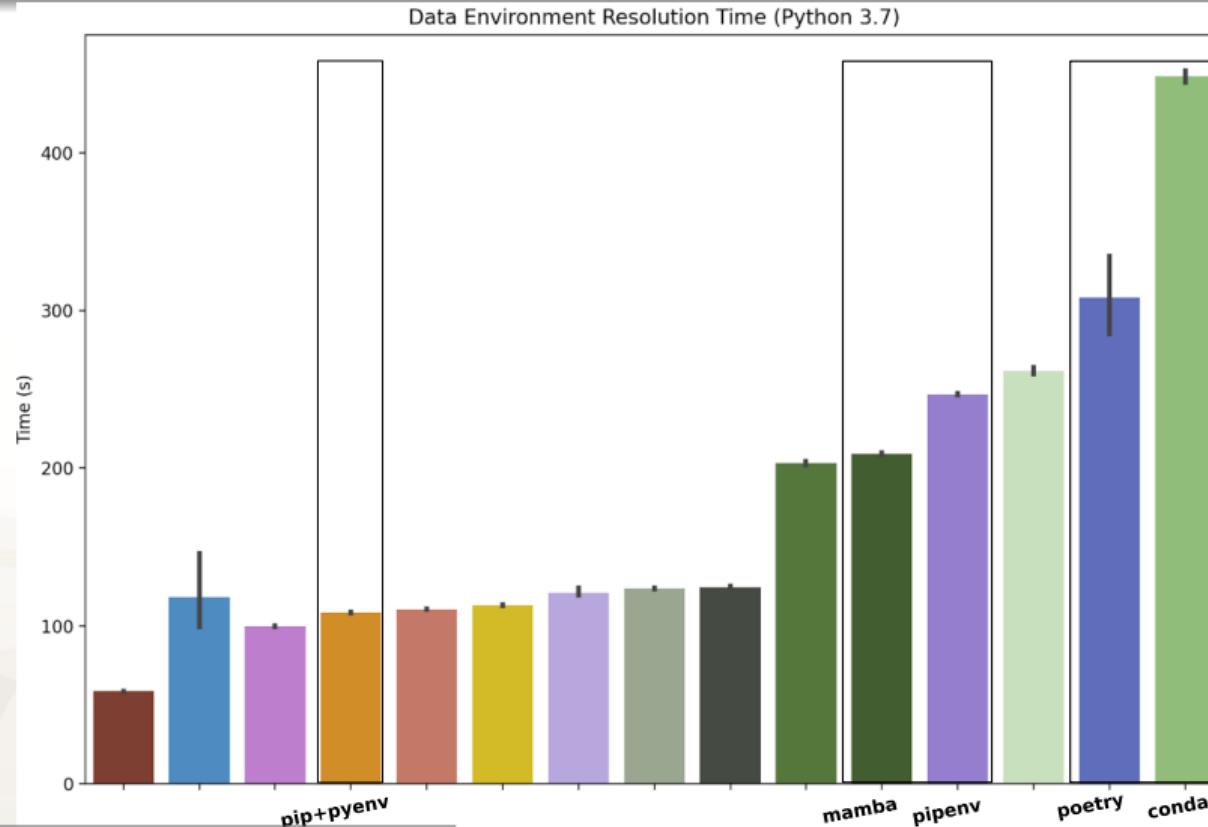
```
$ conda remove bowtie2
```

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 : 

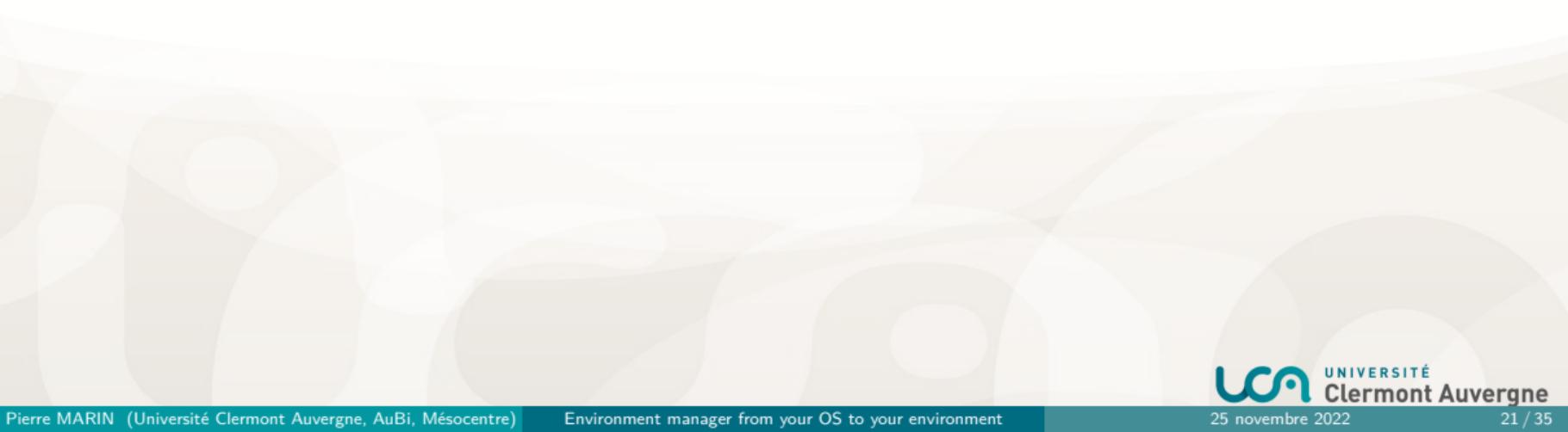
Solomon Hykes was inspired by container port in the world travel



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

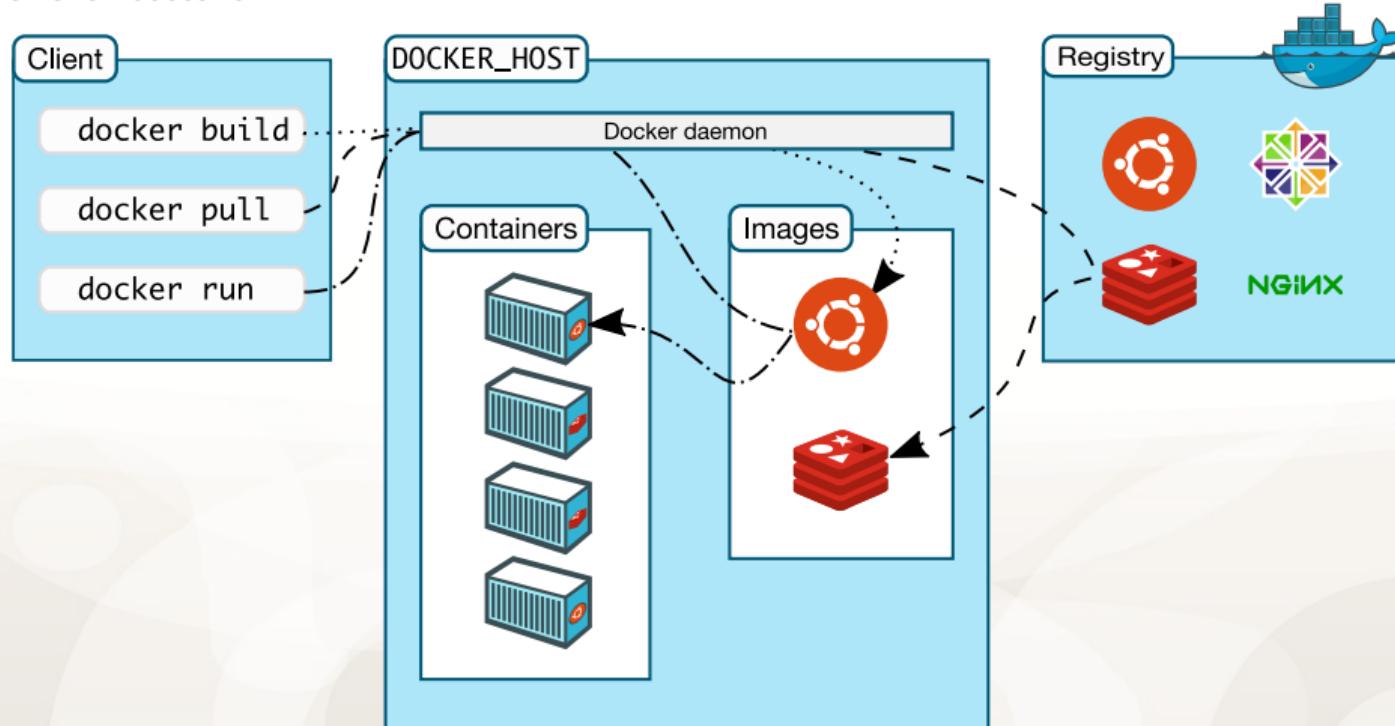
- Set of libraries, functions
 - Static state
 - Online Store or share
 - Automatically build

- Docker container → instance of an image

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

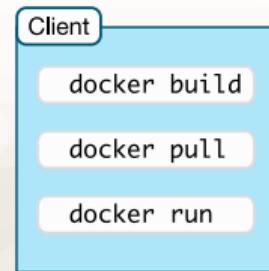
Docker architecture

client-server architecture



Docker client

1 Client to interact with Docker

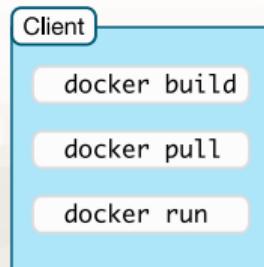


Docker client

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

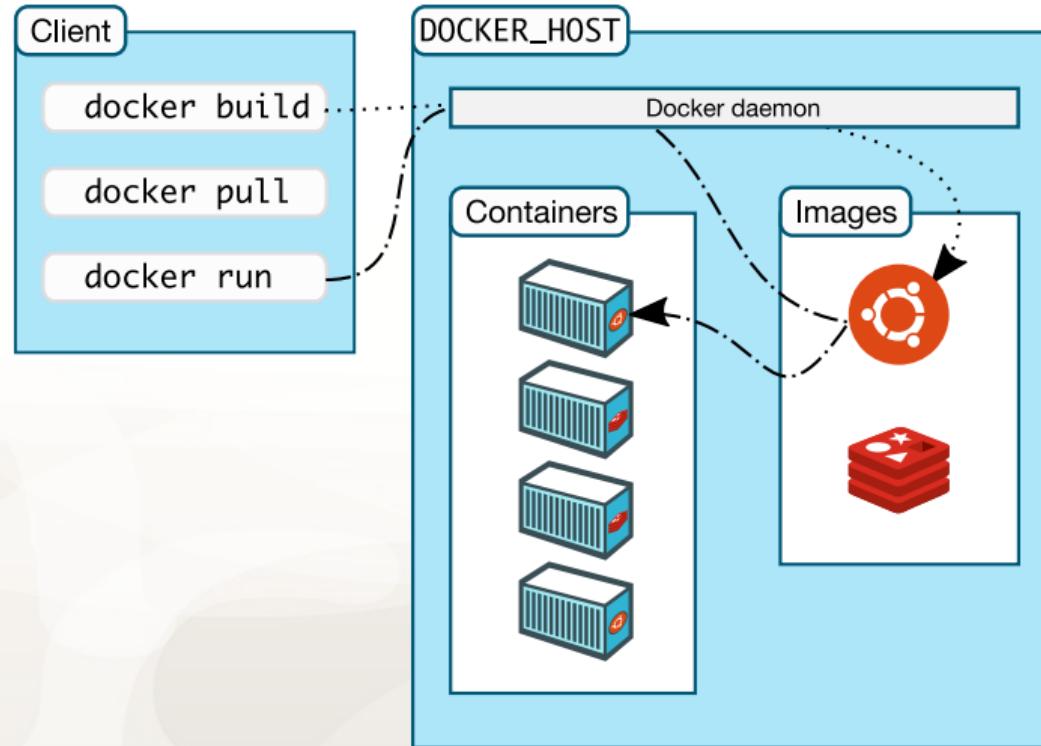
Client

```
$ 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
```



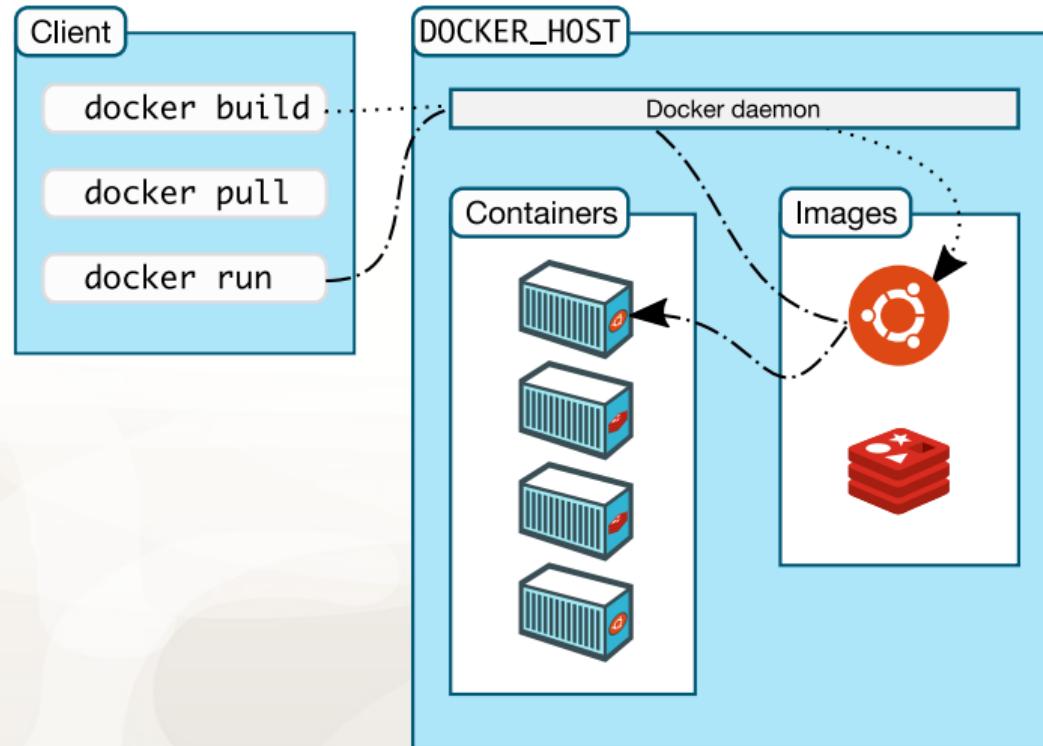
Docker daemon

- 1 Listen client requests



Docker daemon

- 1 Listen client requests
- 2 Manage Docker 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'. The main content area displays search results for 'rstudio'.

Filters:

- Images
- Extensions
- Plugins
- Docker Official Image
- Verified Publisher
- Sponsored OSS

Products:

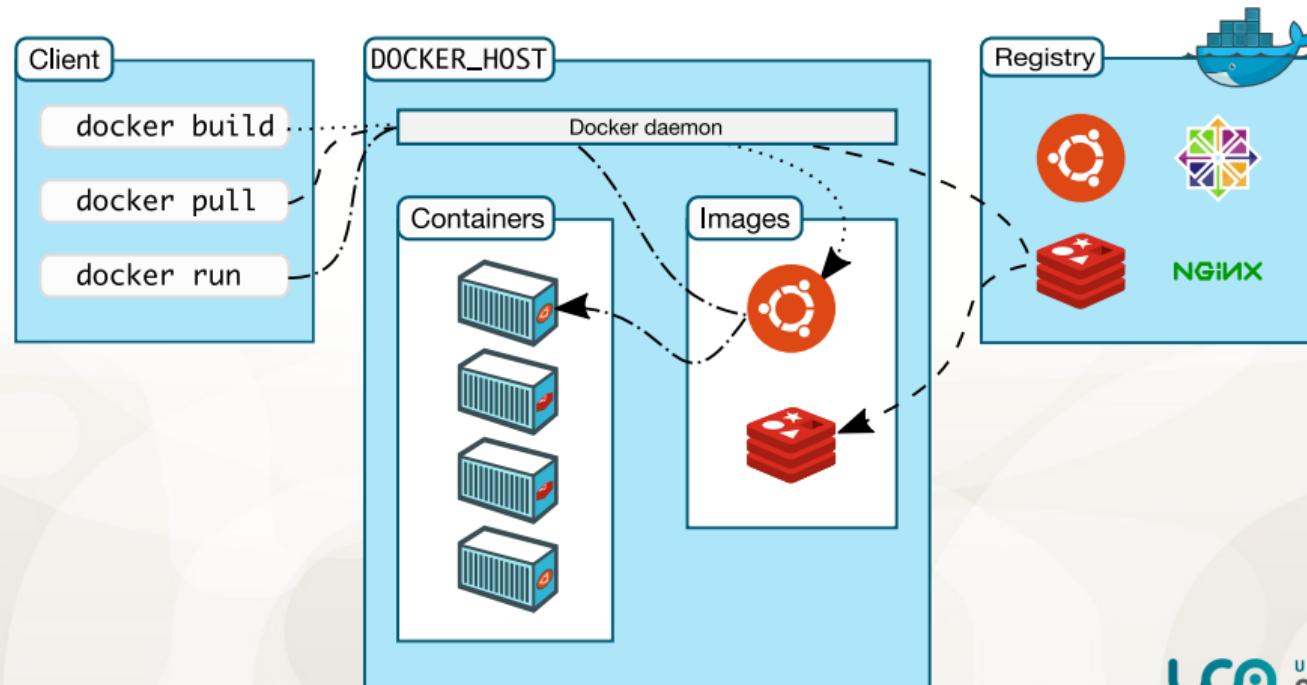
- 1 - 25 of 2 123 results for **rstudio**.
- Best Match

Results:

- ibmcom/rstudio-ppc64le** (Verified Publisher)
By IBM • Updated 3 years ago
Integrated development environment (IDE) for R
Linux ppc64le
521 Downloads 4 Stars
- whoretale/rstudio-base** (Sponsored OSS)
By whoretale • Updated 5 years ago
Linux x86-64
167 Downloads 0 Stars
- bioconductor/rstudio_yescds** (Sponsored OSS)
By bioconductor • Updated 2 months ago
Linux x86-64
62 Downloads 0 Stars

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

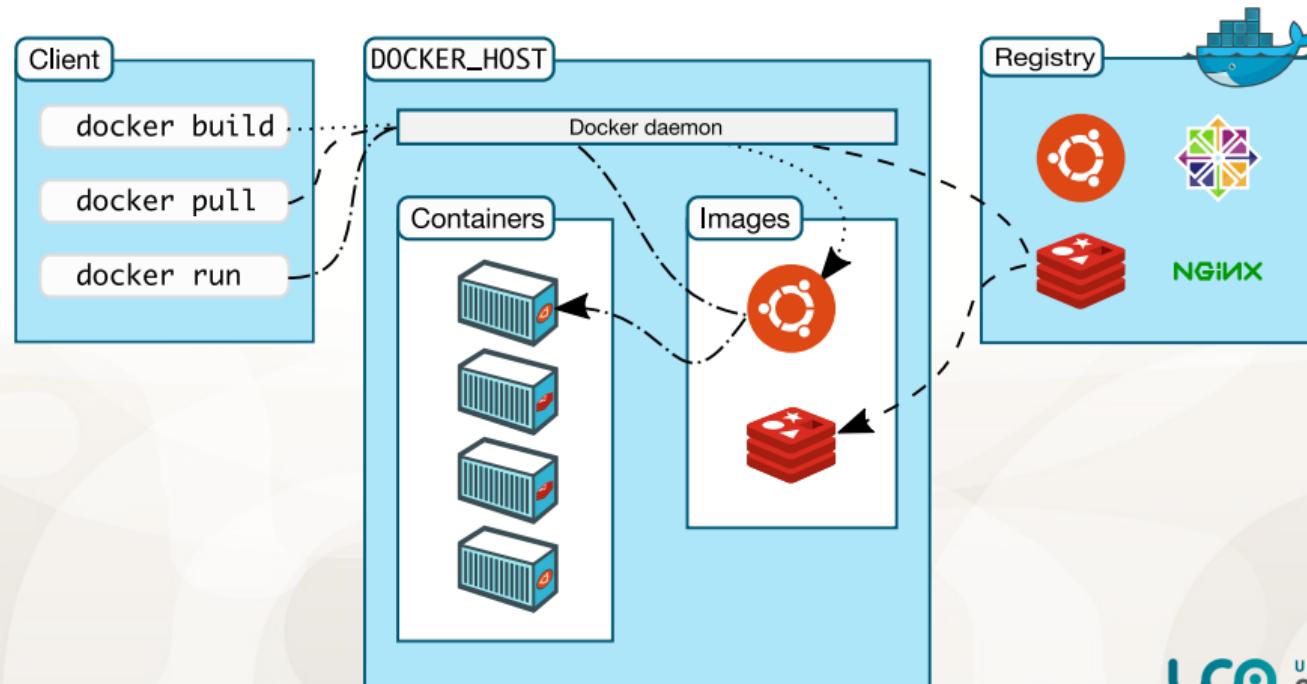


Image layers

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
```

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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- Release in 2015
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- HPC compatible, no root write, integrate ressource managers (slurm)
- Could use Docker images

Singularity commands

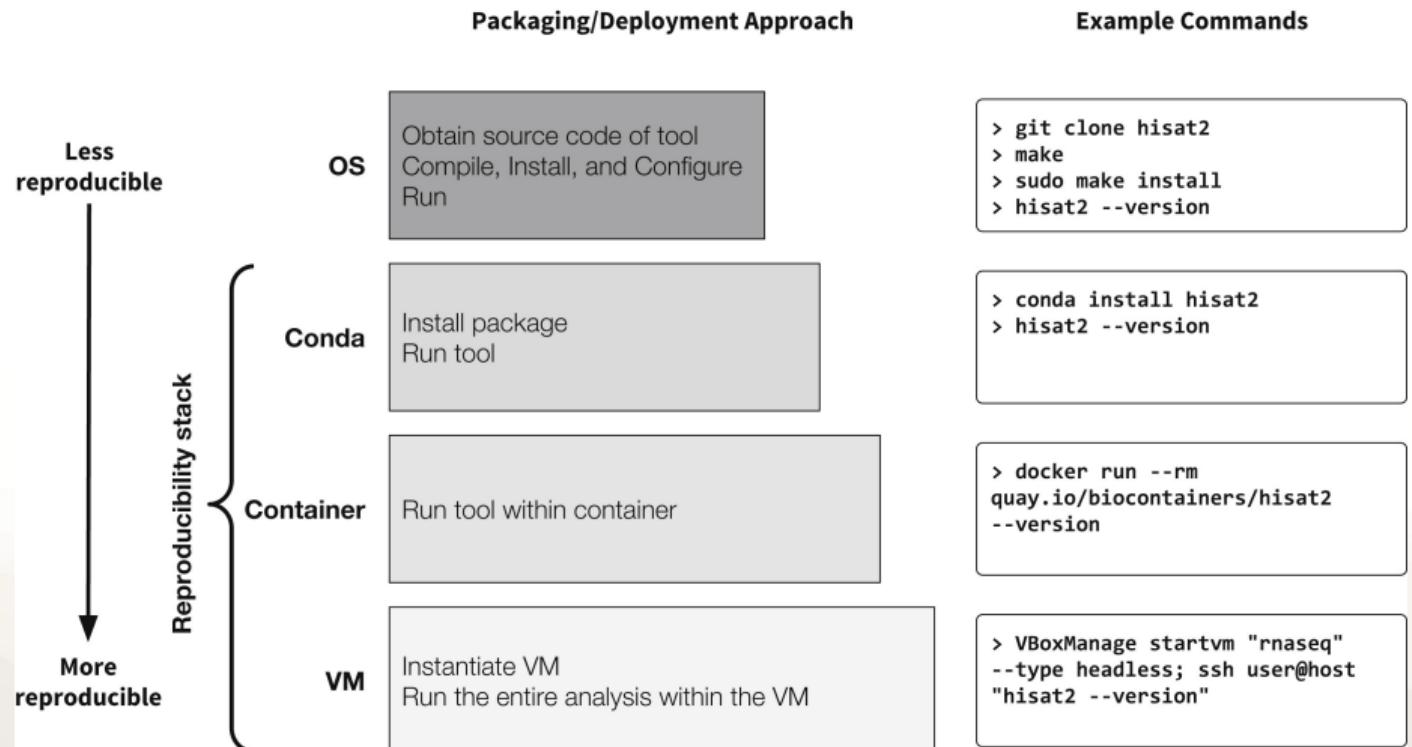
classical commands

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

Singularity and Docker

Singularity can use Docker images

```
$ 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...
```



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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Encapsulation PRACTICE

Conda, Singularity and Docker