Environment manager from your OS to your environment

Encapuslation levels using docker, conda

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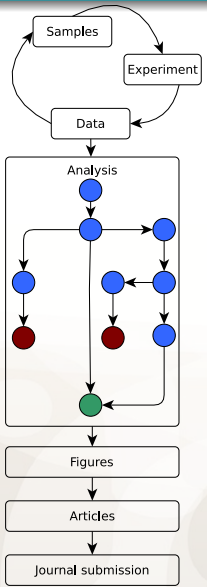
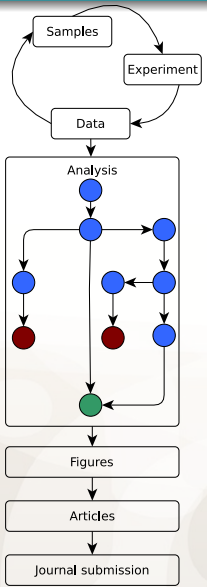
. This work is derived from the IFB and I2BC team members

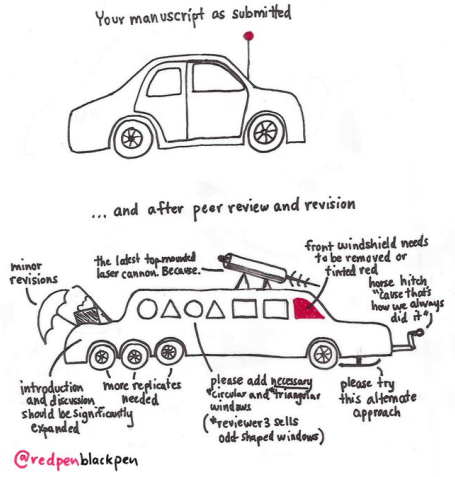
Sommaire

A classic use case



A classic use case





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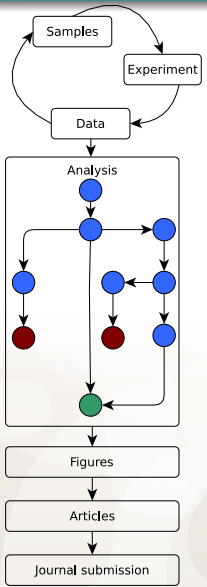

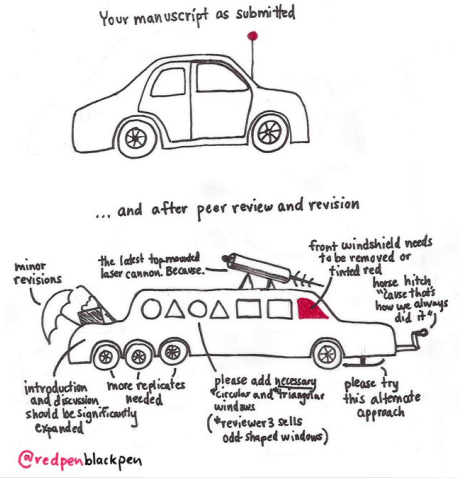

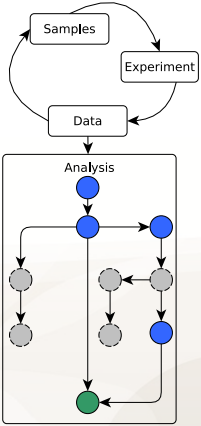

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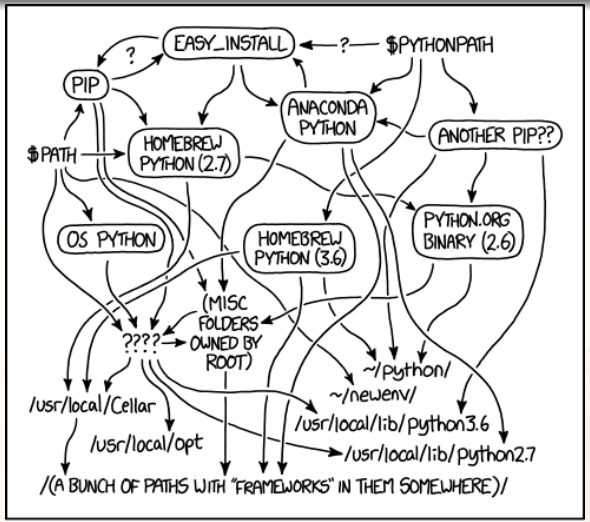
A classic use case

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
  - coexistance bewteen severals versions, libraries

My python env



Encapsulation levels

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

- Hardware virtualisation (virtual machines)

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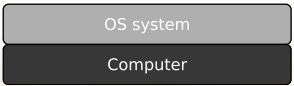
- Environment management (package manager) CONDA

Example of R and package installation

Classical installation

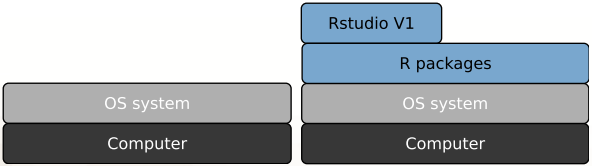
- Start with a computer and a specific OS



Example of R and package installation

Classical installation

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



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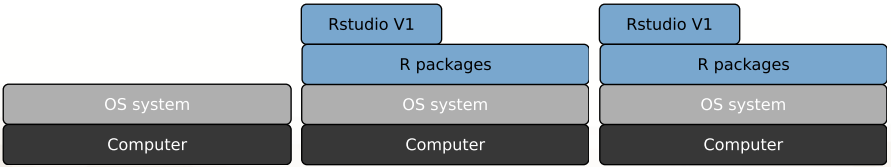

Example of R and package installation

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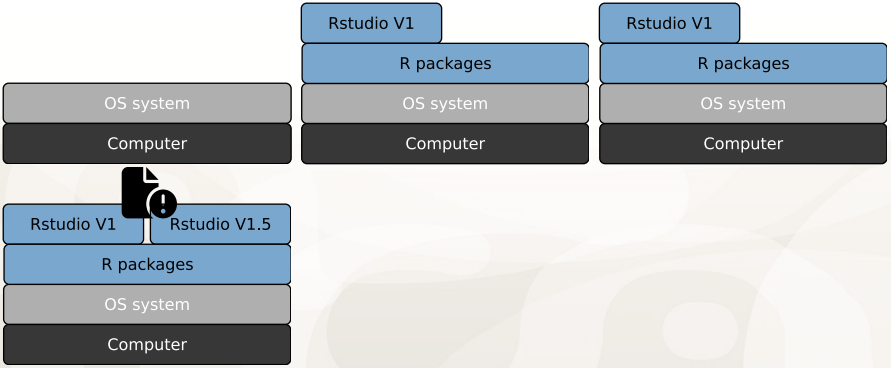
- Start with a computer and a specific OS
- Inside, we installed a new R application
- R need some dependencies
- we tested the last R version –> might be conflicts



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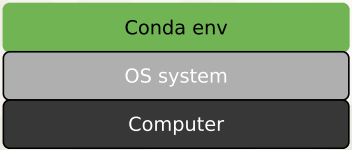
- The idea is to separate each application in here own environment CONDA



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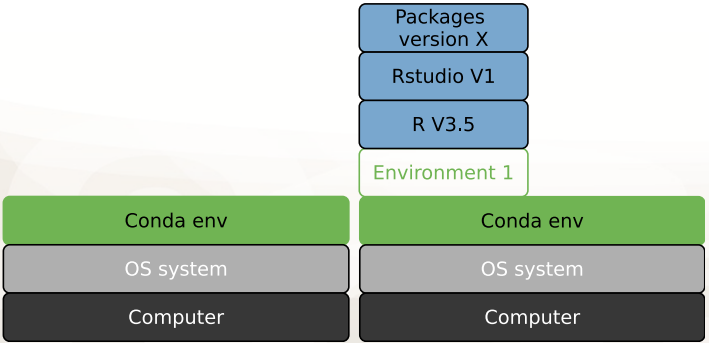
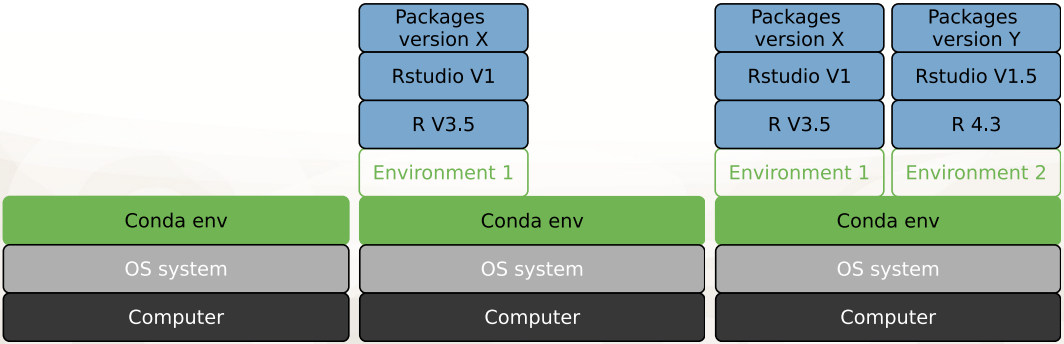


Example of R and package installation

Conda use

- The idea is to separate each application in here own environment CONDA
- A tool version, a conda environment
- Create a new environment for my new tool version, my analysis...



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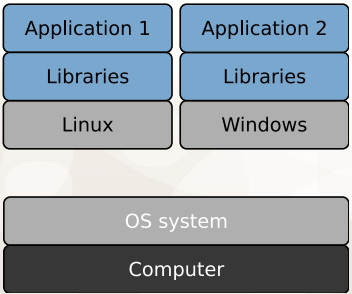
hardware virtualisation

- If we want a software from a different OS ?



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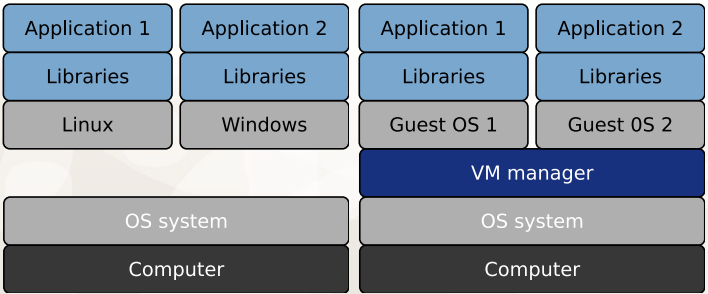
hardware virtualisation

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



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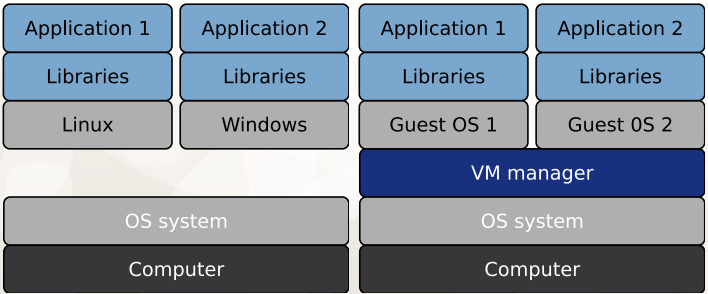
- Each application get a total different and independant environment



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hardware virtualisation

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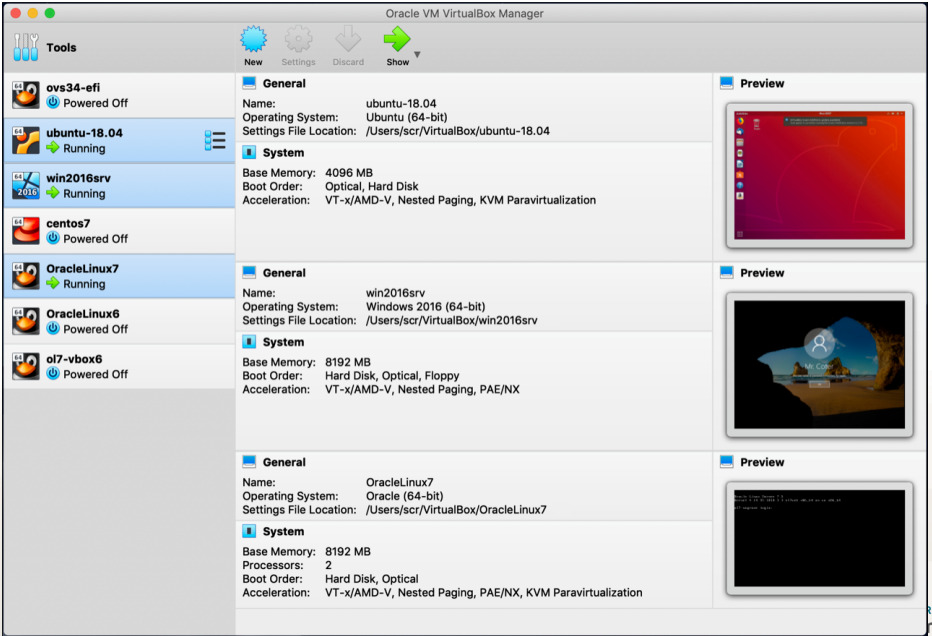
- Redundancy between VMs
- Heavy to set up
- No automation


Oracle VM VirtualBox Manager
Tools
New
Settings
Discard
Show
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

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OS virtualisation

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

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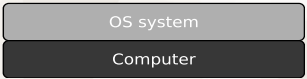
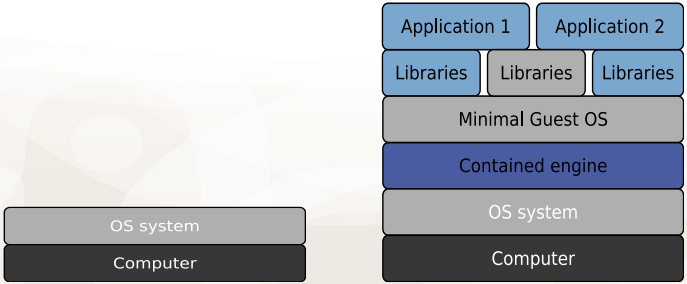


Example of R and package installation

OS virtualisation

- "Trick" applications into believing that they are in a different OS than the host's
- Named containers : docker or
- Avoid redundancy



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- Avoid redundancy
- Speed
  - Faster installation
  - No boot time

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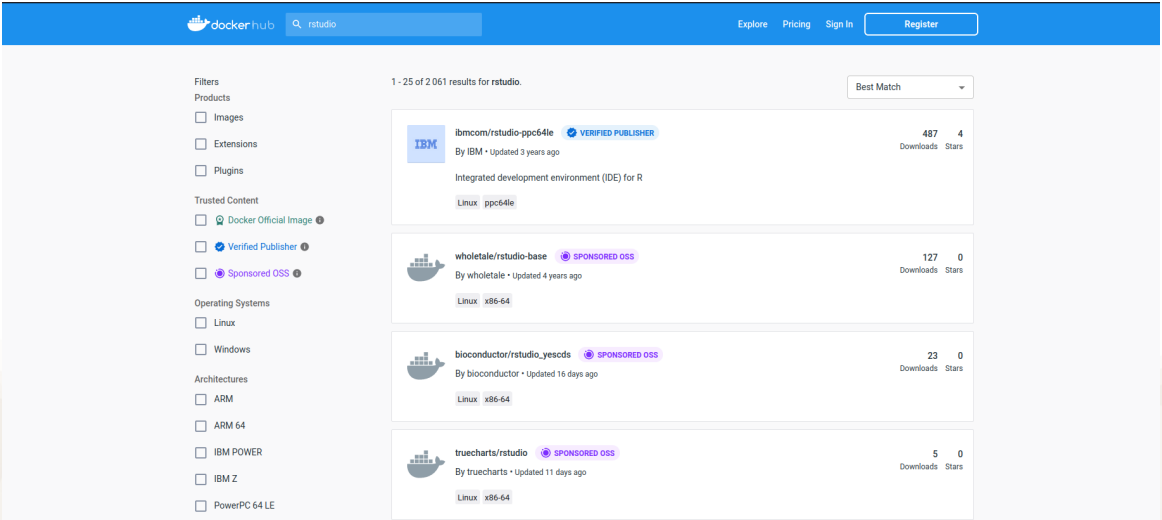
OS virtualisation

- "Trick" applications into believing that they are in a different OS than the host's
- Named containers :  or 
- Avoid redundancy
- Speed
  - Faster installation
  - No boot time
- Lightweight
  - Minimal base OS
  - Minimal set of library and global environment
  - Easy sharing of application


docker hub
rstudio
Explore
Pricing
Sign In
Register
Filters
Products
Images
Extensions
Plugins
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 Downloads
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wholetale/rstudio-base
SPONSORED OSS
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Linux
x86-64
127 Downloads
0 Stars
bioconductor/rstudio_yescds
SPONSORED OSS
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0 Stars
truecharts/rstudio
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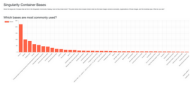
By truecharts • Updated 11 days ago
Linux
x86-64
5 Downloads
0 Stars

Singularity Community Catalog

About



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 policies

Conda system

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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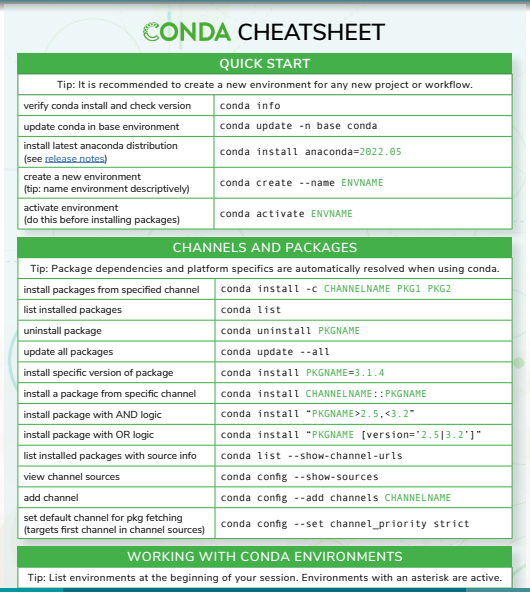
  - Same advantages ad Anaconda
- Conda CONDA
  - Package manager AND environment manager
  - installed with Ana or Miniconda
  - Python based but can also install tools from R, C++ or Julia...

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=2022.05`
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

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- R
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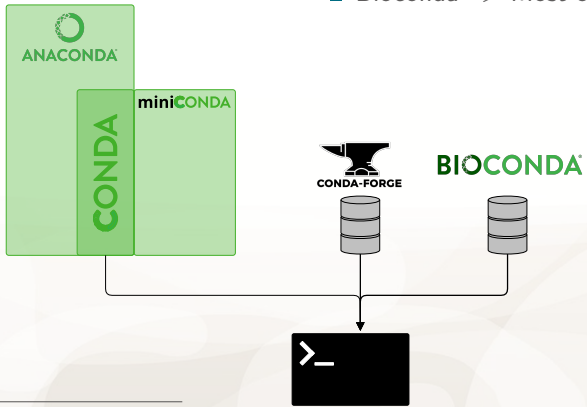

. Bioconda : sustainable and comprehensive software distribution for the life sciences *Grüning et al.*, Nature methods, 2018. DOI 10.1038/s41592-018-0046-7

Basic commands

Create environment

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$ conda create -n [env_name]
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$ conda search bowtie2

$ conda search -c bioconda bowtie2

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Install tools

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$ conda install -c bioconda bowtie2=2.4.5

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Install tools

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Remove tools

$ conda remove bowtie2

Environment resolution

Conda also manage your environment to install compatible tools in the same environment

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- time to solve the environement installation plan
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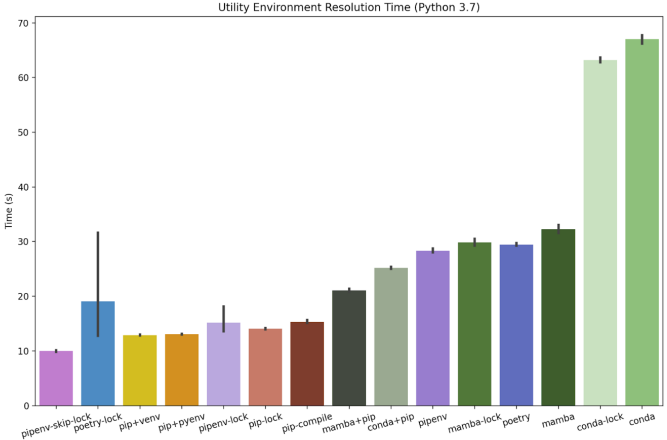
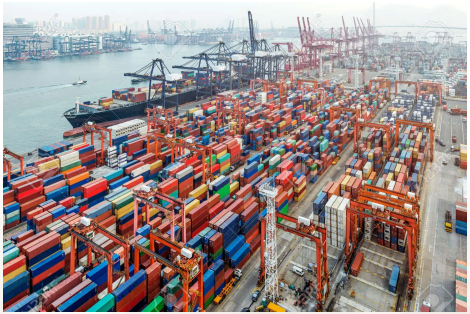


Container technology is not very old

The most famous : docker

Solomon Hykes was inspirated 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

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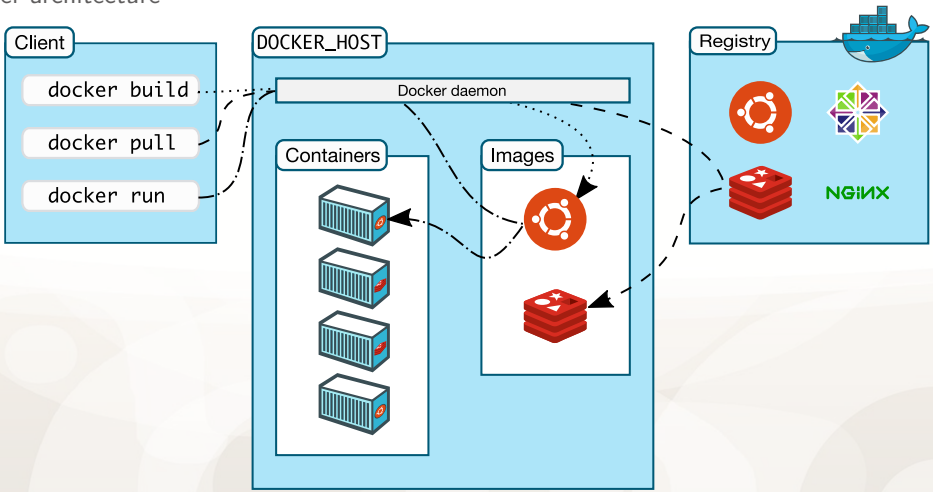
- Docker container –> instance of an image
  - Result of the image activation
  - Can be modified
  - Can be tunred into an image
  - 1 image –> multiple containers

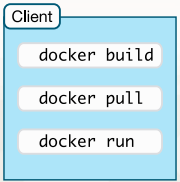
Docker architecture

client-server architecture



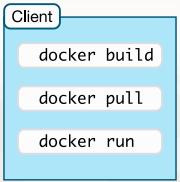
Docker client

1. The user way to interact with Docker



Docker client

1. The user way to interact with Docker
2. Client talk to a daemon (Docker background program)

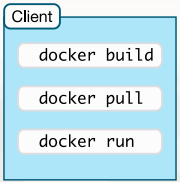


Docker client

1. The user way to interact with Docker
2. Client talk to a daemon (Docker background program)
3. API based –> can communicate with several deamons

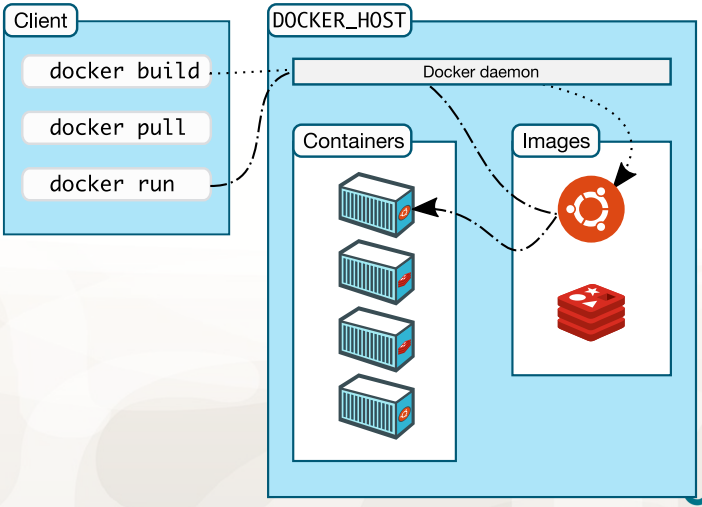
Client

```
$ 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
```



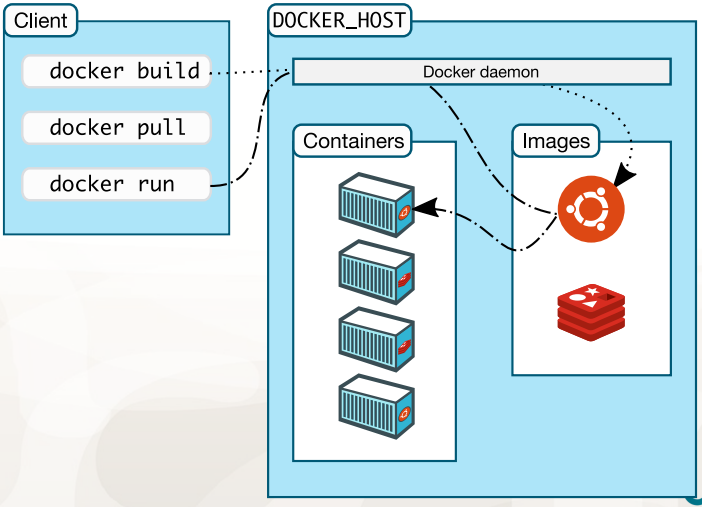
Docker daemon

1. listen API requests



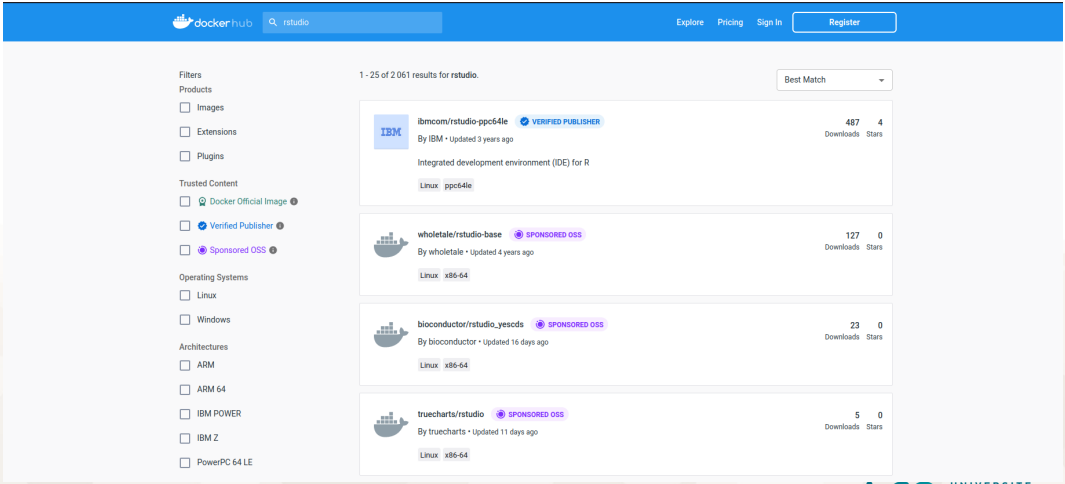
Docker daemon

1. listen API requests
2. manage Dockers images, containers...



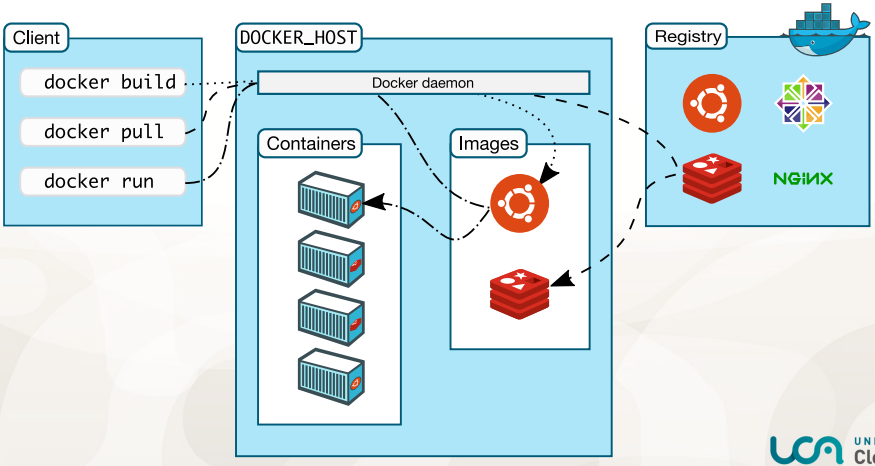
Docker registries

1 Store Docker images



Docker registries

1. Store Docker images
2. Docker hub is a publix registry



Docker registries

1. Store Docker images
2. Docker hub is a publix registry
3. You can run your own registry

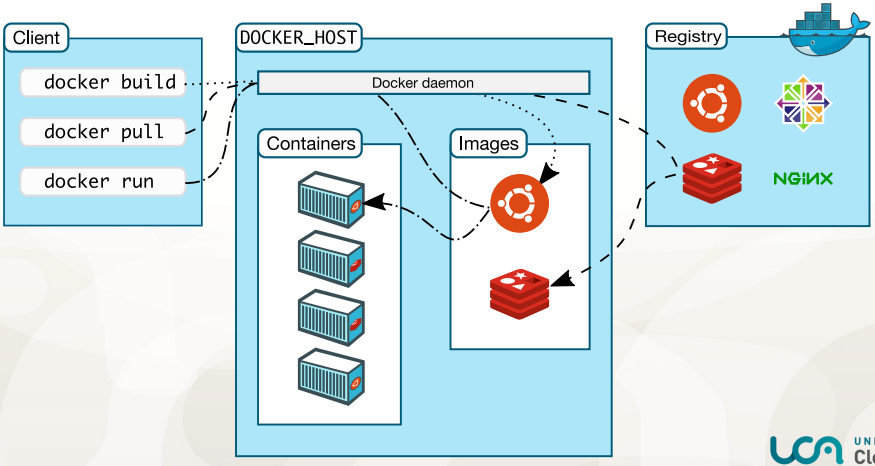


Image layers

Focus on image building

- Layers building

```
$ 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
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- Several layers to one image

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Focus on image building

- Layers building
- Several layers to one image
- Some layers shared by images when pulling

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- Lightheight the download and use of image on you computer

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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.

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

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

Singularity commands

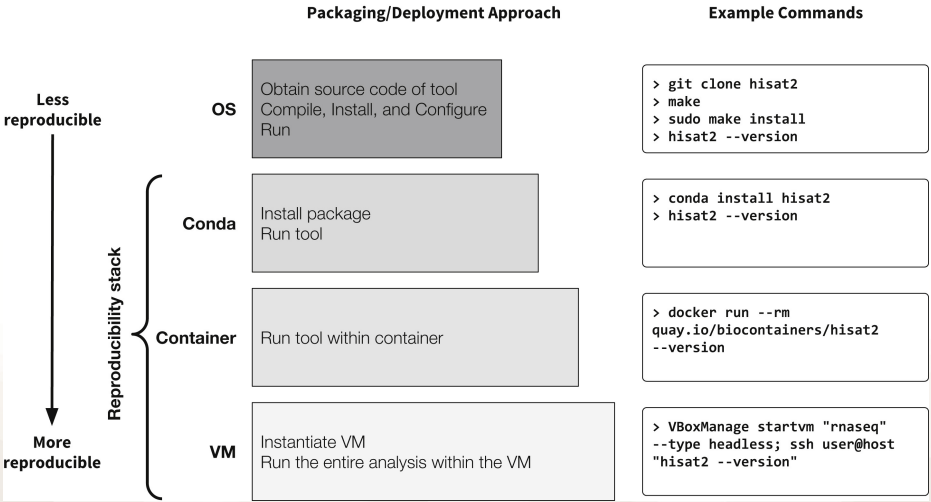
classical commands

```
$ 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 10.1016/j.cels.2018.03.014

Some recommandations

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. Recommendations for the packaging and containerizing of bioinformatics software Gruening, F1000 Research, 2019. DOI 10.12688/f1000research.15140.2

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- Provide helpful usage message

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