Environment manager from your OS to your environment

Encapuslation levels using docker, conda [1]

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

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   - The use of packaging
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2. Manage your local environment
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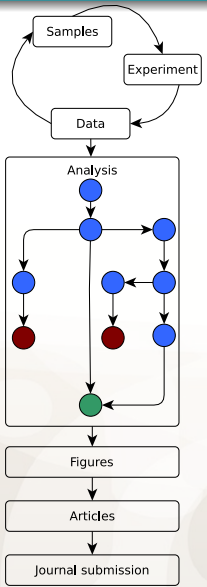
4. Manage your OS configuration
   - How container works
5. Conda ecosystem
   - a case of bioconda
6. A second level, the containers
   - Docker
   - Singularity

A classic use case



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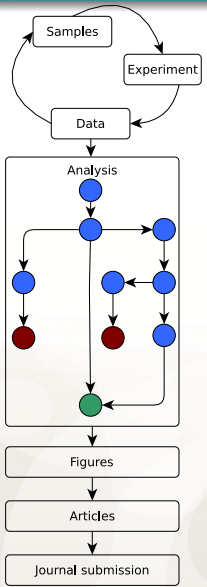

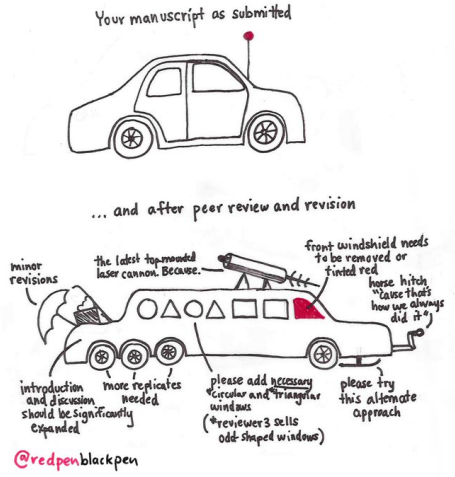

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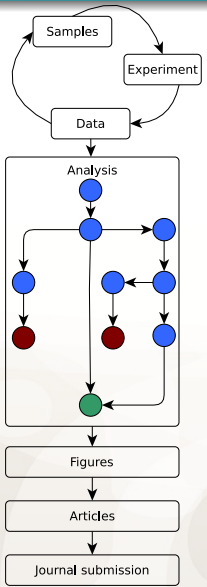
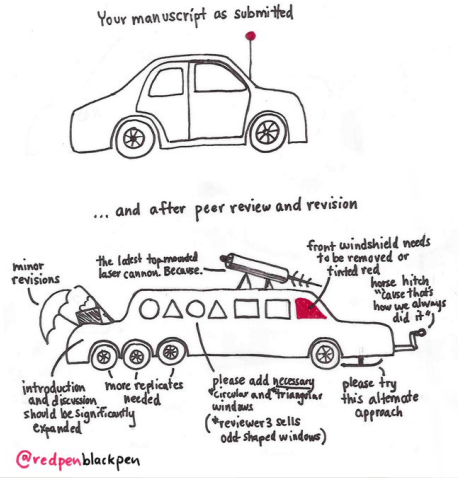
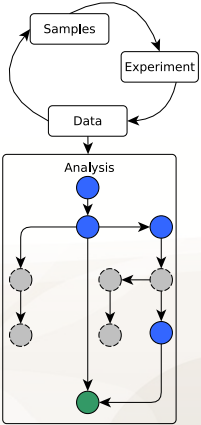






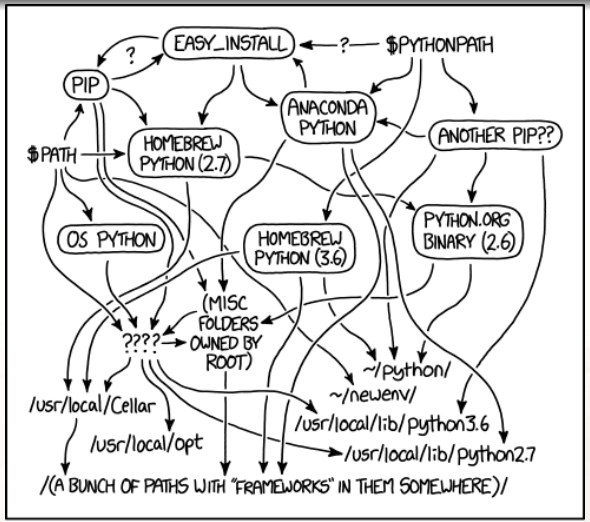
A classic use case

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



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Encapsulation levels

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

- Hardware virtualisation (virtual machines)

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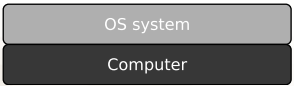
- Environment management (package manager) CONDA

Example of R and package installation

Classical installation

- Start with a computer and a specific OS



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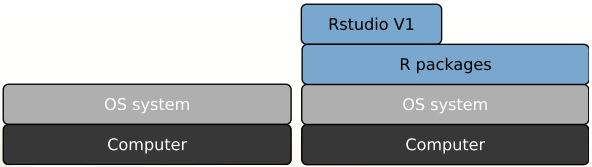

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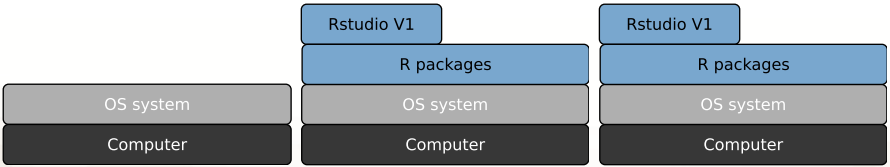

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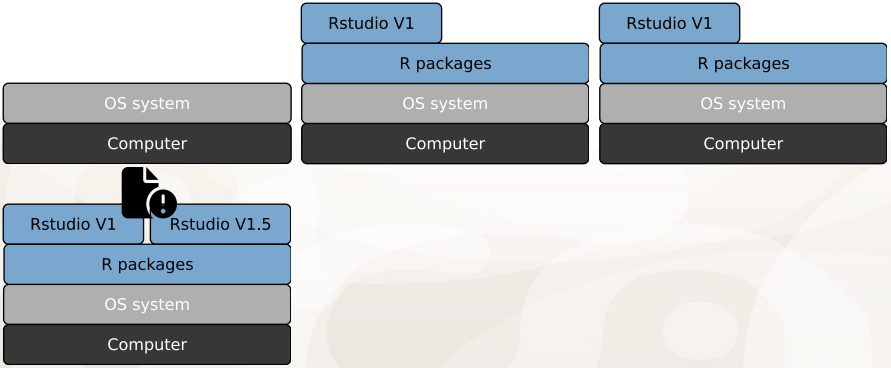
- we tested the last R version –> might be conflicts



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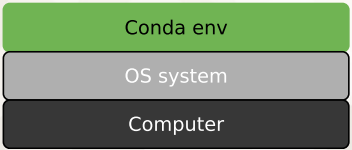

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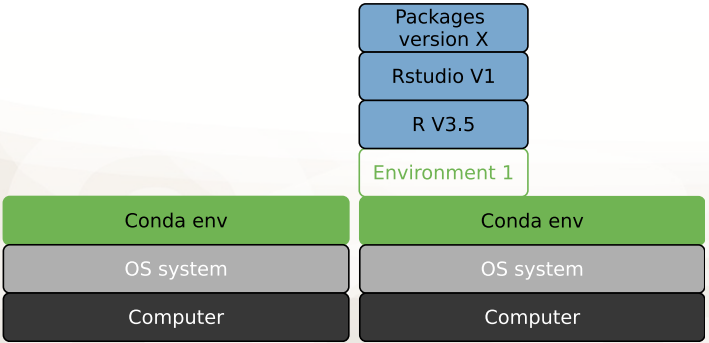

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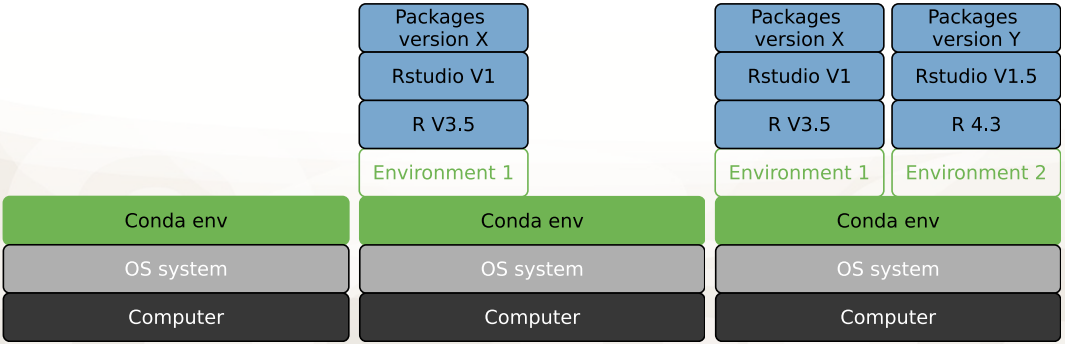
- A tool version, a conda environment
- Create a new environment for my new tool version, my analysis...



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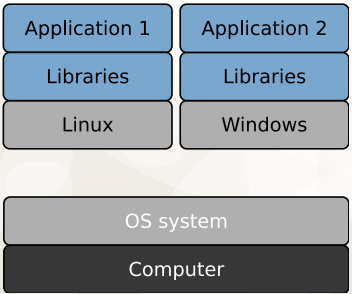
- If we want a software from a different OS ?



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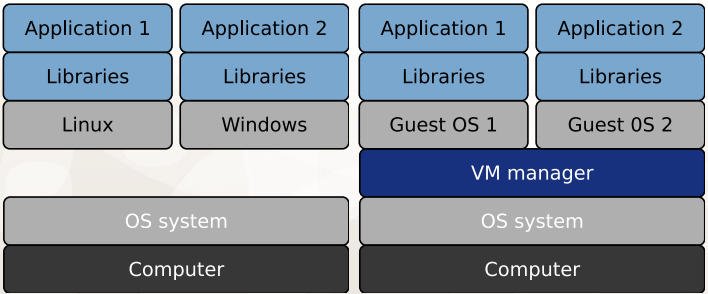
- If we want a software from a different OS ?
- Use virtual machines



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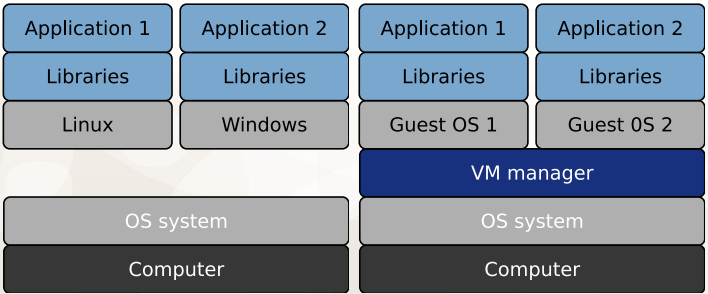

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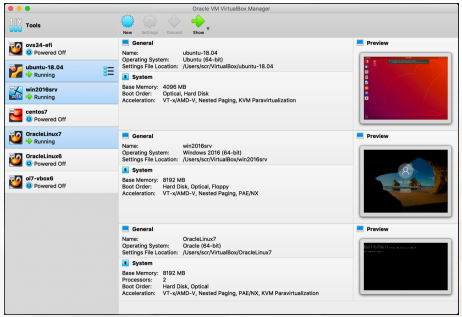

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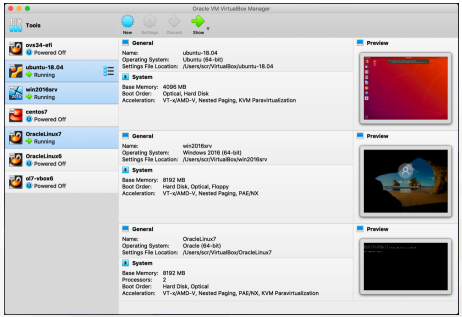

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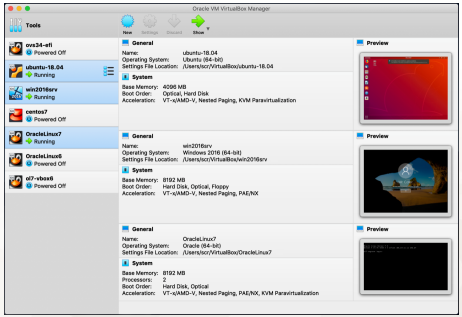

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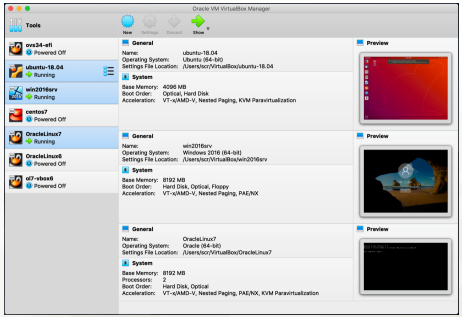

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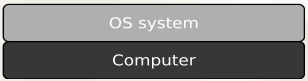

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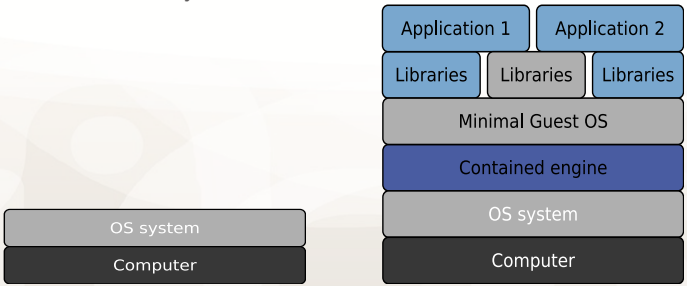

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  - Minimal set of library and global environment
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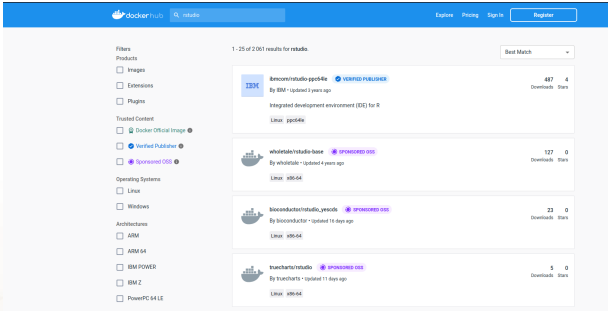

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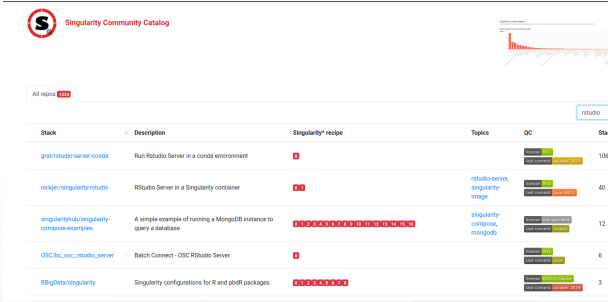

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Example of R and package installation

Helping developers manage inactive images

To help Docker economically scale its infrastructure to support free services for our growing base of users, several updates were announced. First, a new inactive image retention policy was introduced that will automatically delete images hosted in free accounts that have not been used in 6 months. In addition, Docker will also be providing tooling, in the form of a UI and APIs, that will allow users to more easily manage their images. Together, these changes will allow developers to more easily clean up their inactive images and also ensure Docker can economically scale its infrastructure.

With this new policy, starting on **November 1**, images stored in free Docker Hub repositories that have not had their manifest pushed or pulled in the last 6 months will be removed. This policy does not apply to images stored by paid Docker Hub subscription accounts, Docker Verified Publishers , or Docker Official Images.

- **Example #1:** Molly, a free Docker Hub user, pushed a tagged image `molly/hello-world:v1` to Docker Hub on January 1, 2019. The image was never pulled since it was pushed. This tagged image will be considered inactive beginning November 1, 2020 when the new policy takes effect. The image and any tag pointing to hit, will be subject to deletion on November 1, 2020.
- **Example #2**: Molly has another untagged image `molly/myapp@sha256:c0ffee` that was first pushed on January 1, 2018. This image was last pulled on August 1, 2020. This image will be considered an active image and will not be subject to deletion on November 1, 2020.

Minimizing impact to the developer community

For free accounts, Docker offers free retention of images inactive for six months. For users that need their inactive images to be retained, Docker also offers unlimited image retention as a feature of the Pro and Team plans. Visit docker.wpsitekeep.com/pricing to view the available plans.

In addition, Docker will be offering a set of tools and services to help developers easily view and manage their images, including the following product updates which will be made available on Docker Hub in the coming months:

- Image management dashboard to view and manage images across all repositories within a namespace (roadmap issue #146)
- Email notifications for images that are set to expire (roadmap issue #147)
- Restoration of recently deleted images (roadmap issue #148)

2

- No easy use on a cluster system
- Docker private company policies

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Conda system

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  - Open source distribution
  - Cross platform
  - Available on cluster without admin whrite
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- 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**

3. 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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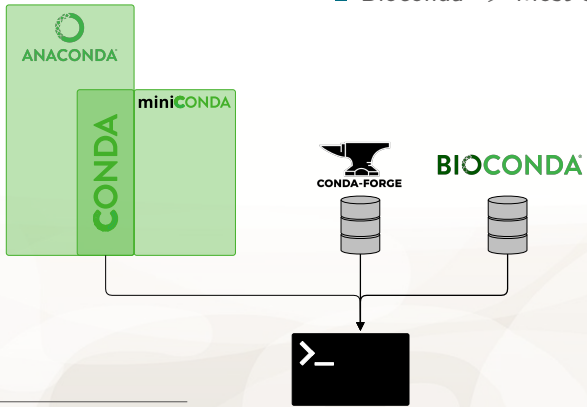

3

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Basic commands

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Remove tools

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Environment resolution

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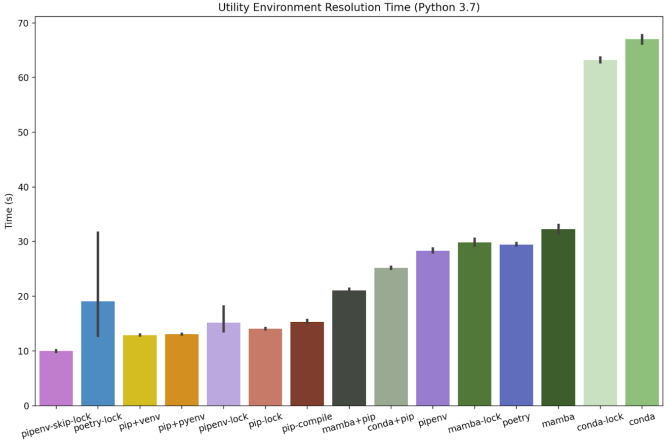

Container technology is not very old

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

- Born in 2010
- First public release in 2013

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- V 1.0 in 2014
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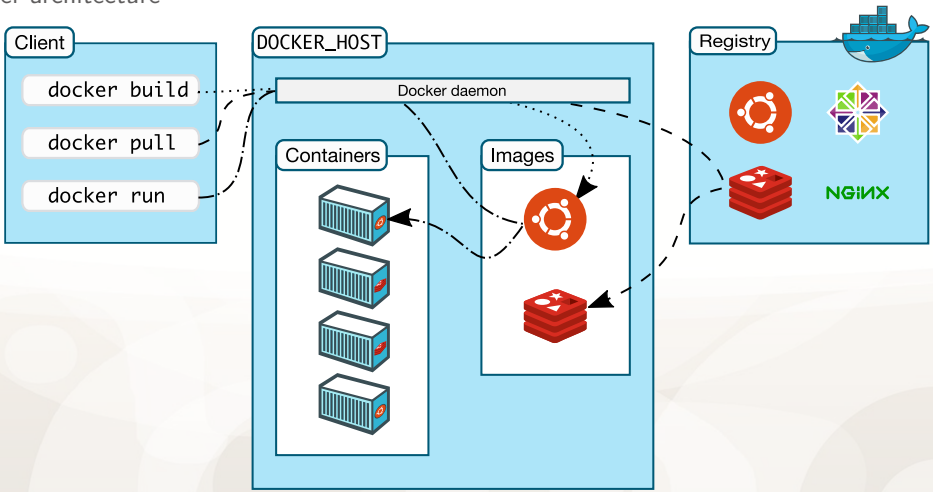
- Packaged to Ubuntu in 2014 (V14.04)

[<+->]Term definitions

- Docker image –> "snapshot" immutable file
  - Set of libraries, functions
  - Static state
  - Online Store or share
  - Automatically build
- Docker container –> instance of an image
  - Result of the image activation
  - Can be modified
  - Can be tunred into an image
  - 1 image –> multiple containers

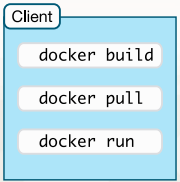
Docker architecture

client-server architecture



Docker client

1. The user way to interact with Docker



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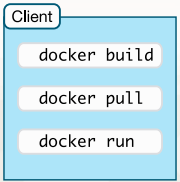
1. The user way to interact with Docker
2. Client talk to a daemon (Docker background program)



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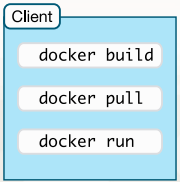

Docker client

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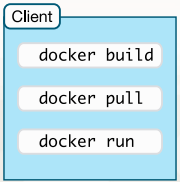
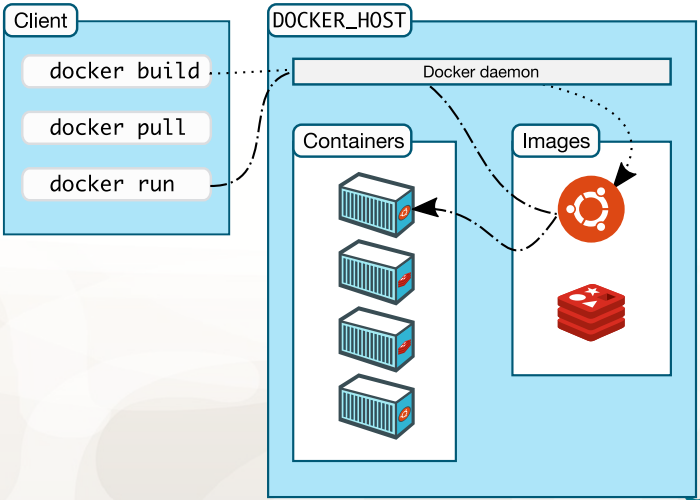
Client

```
$ 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
```



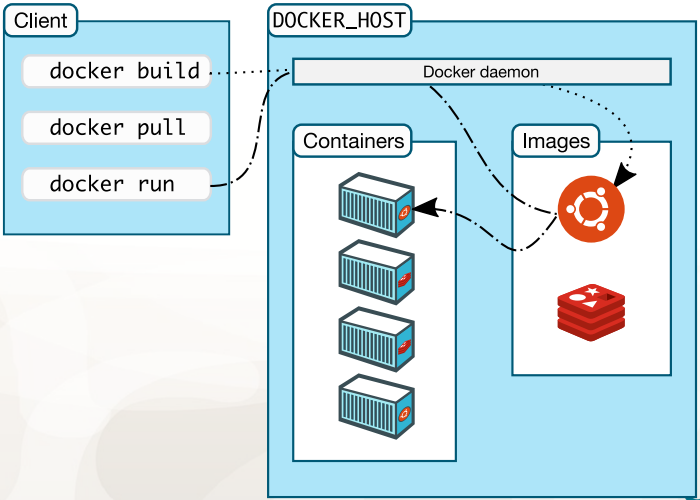
Docker daemon

1. listen API requests



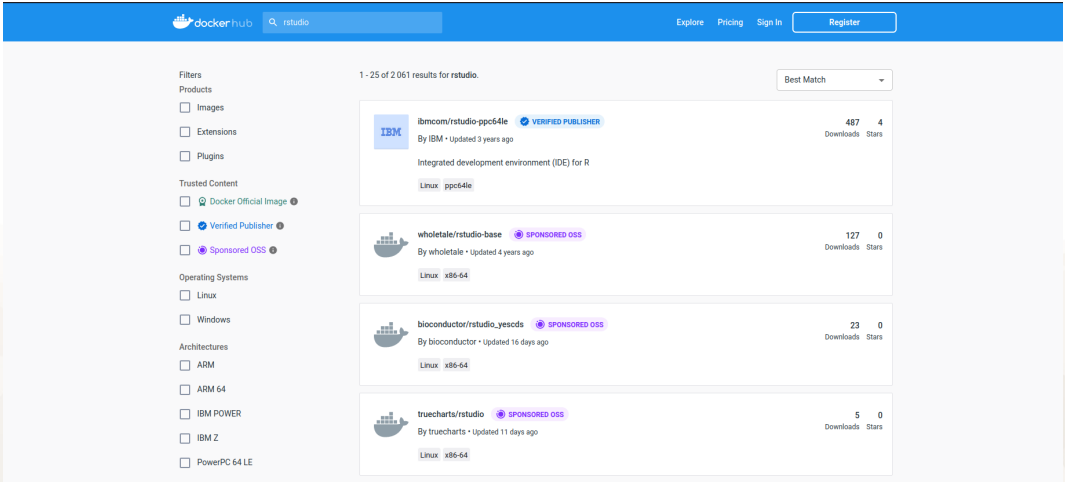
Docker daemon

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



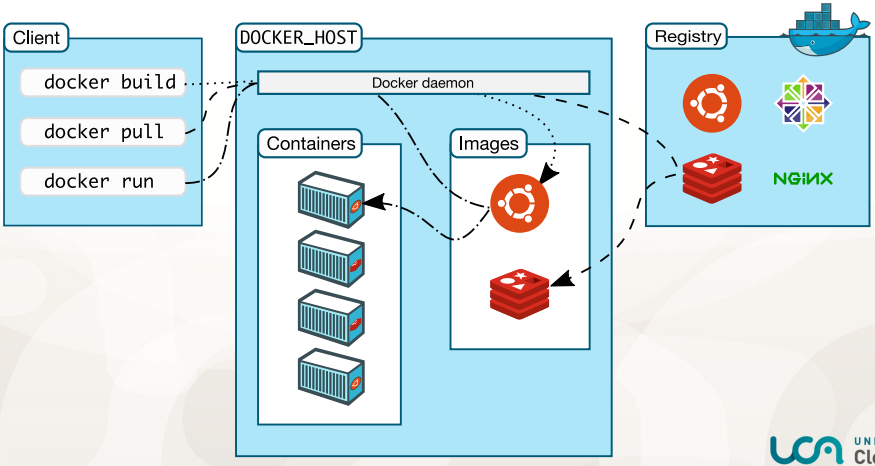
Docker registries

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

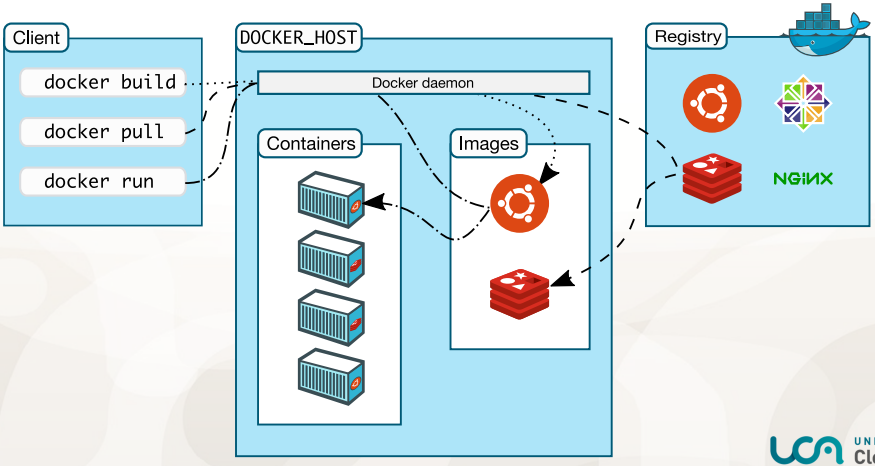


Image layers

Focus on image building

- Layers building

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

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- Lightheight the download and use of image on you computer

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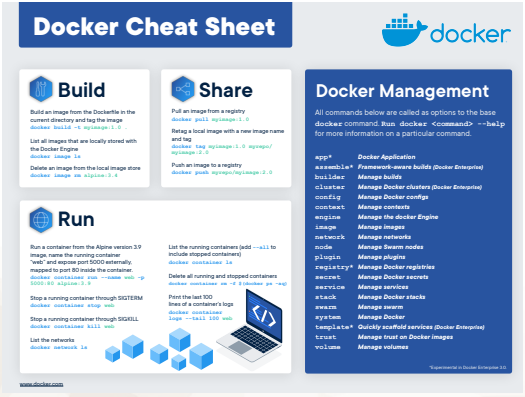

DOCKER COMPOSE CHEAT SHEET

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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- More adopted in Academic institutions
- 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

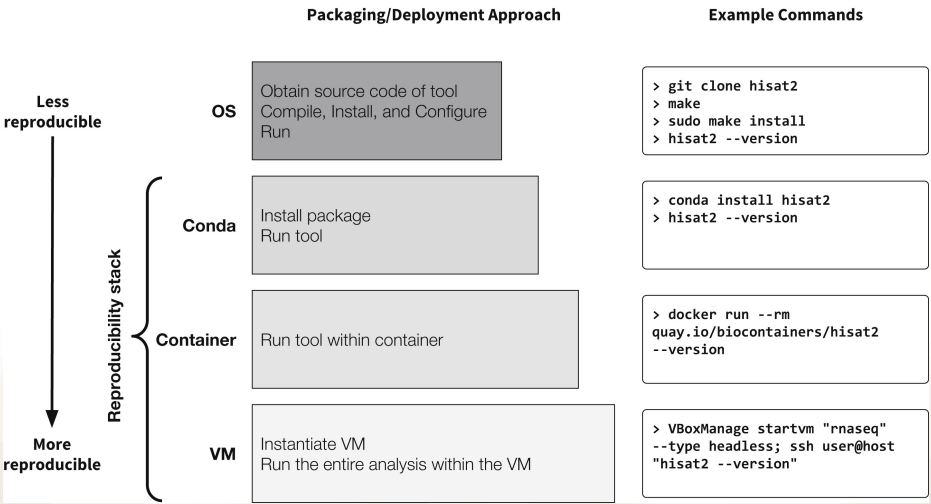
classical commands

```
$ 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...
```



4

4. Practical Computational Reproducibility in the Life Sciences Grüning et al, Cell Systems, 2018. DOI 10.1016/j.cels.2018.03.014

Some recommandations [5]

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