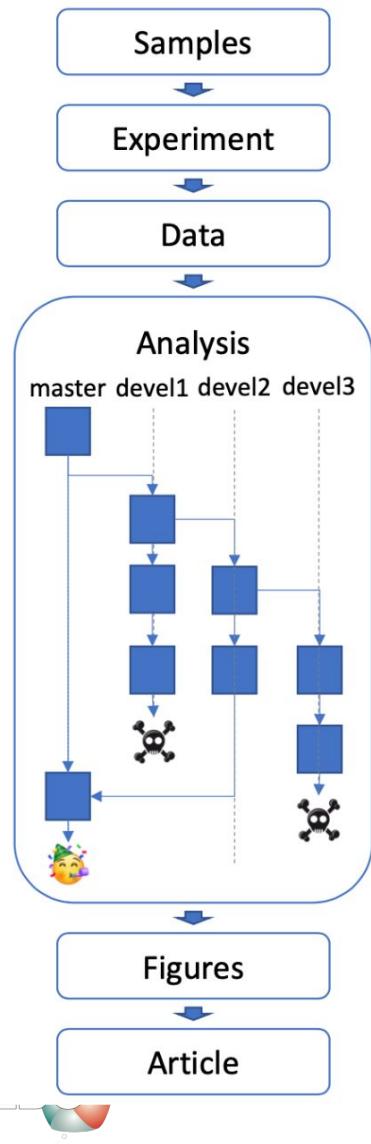


# Use case 2 : Encapsulation

Céline Hernandez, I2BC, 0000-0001-8664-1340

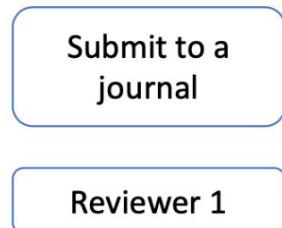
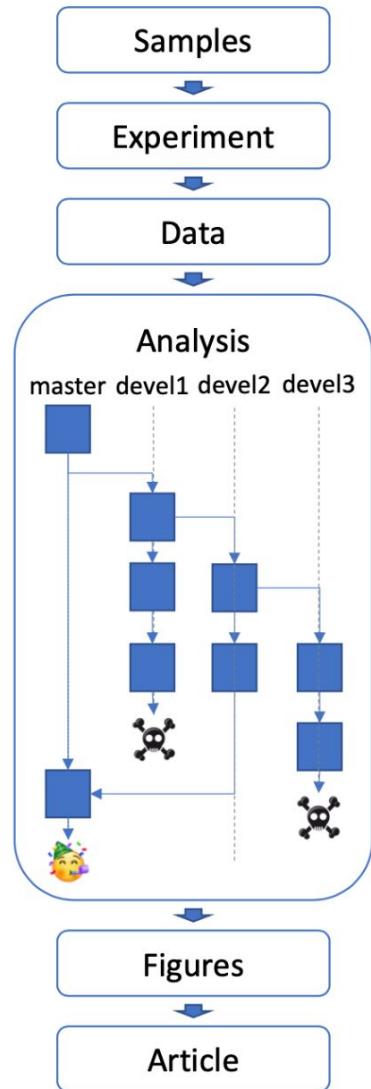


## A (not-so-uncommon) nightmare

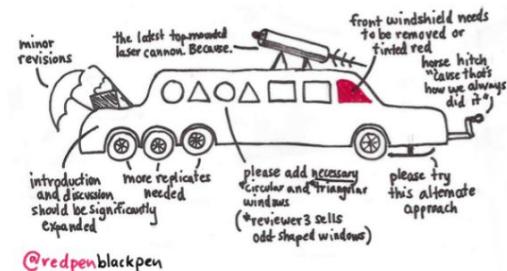




## A (not-so-uncommon) nightmare



Reviewer 2

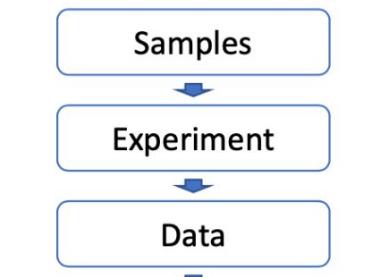


Reviewer 3

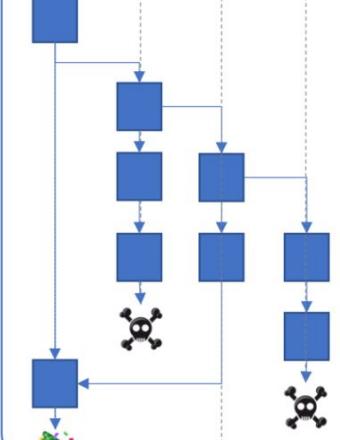




## A (not-so-uncommon) nightmare

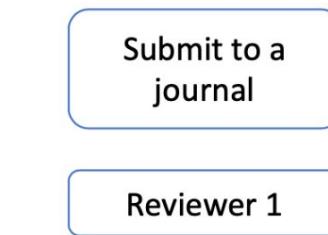


Analysis  
master devel1 devel2 devel3

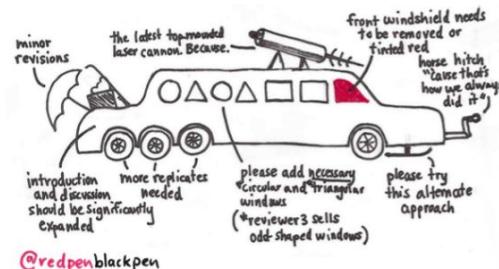


Figures

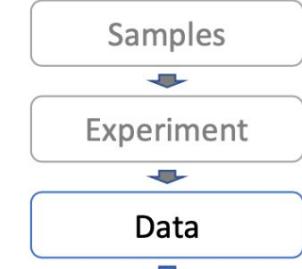
Article



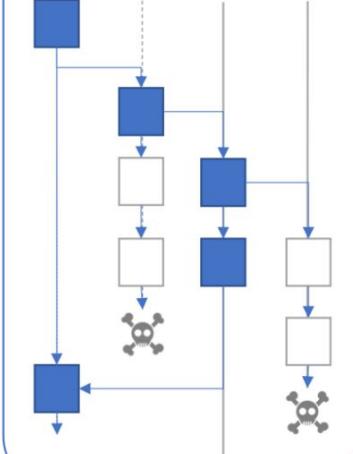
Reviewer 2



Reviewer 3

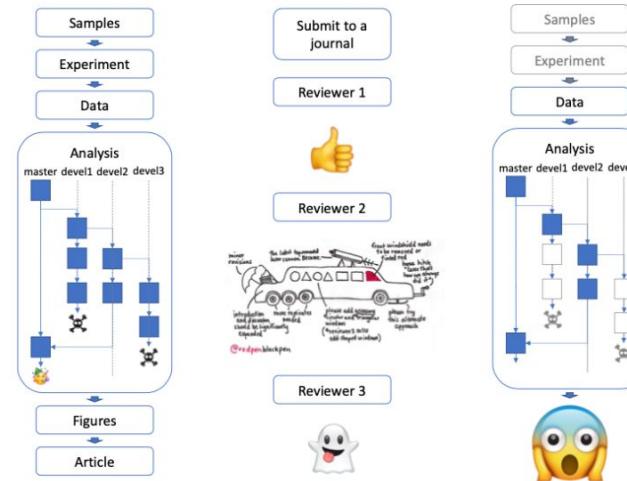


Analysis  
master devel1 devel2 devel3





## A (not-so-uncommon) nightmare



What changed?

- Package
- Software
- Libraries
- Environment variables
- OS version
- Computer
- ...?



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

- Hardware virtualisation (virtual machines) 
- OS virtualisation (images and containers) 
- Environment management 



## Let's say we want to install RStudio...

### Install Rstudio ?

The screenshot shows the RStudio website at <https://www.rstudio.com/ide/download/>. The main heading is "Download the RStudio IDE". Below it, there's a section titled "Choose Your Version" with a note about the IDE being a set of integrated tools for R and Python. It includes a "Learn more about RStudio Team" button and a small image of the RStudio team.

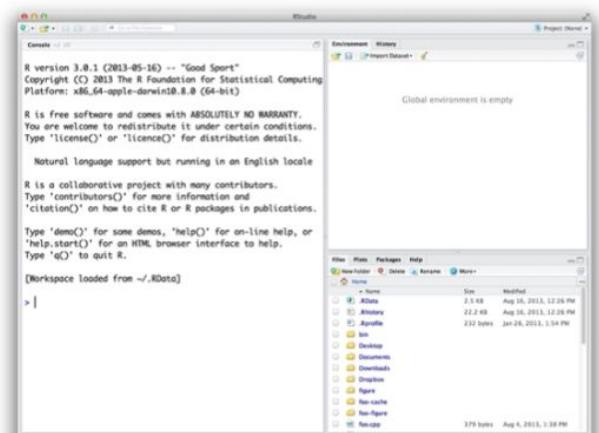
### MacOS



### Windows



### Use Rstudio

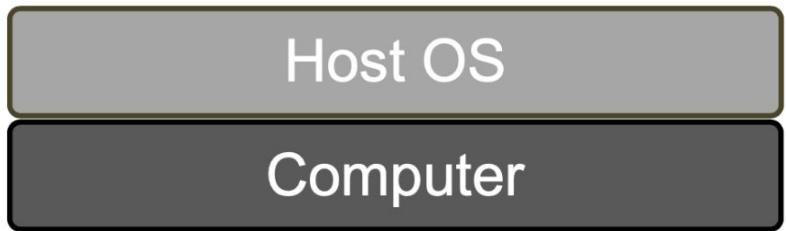


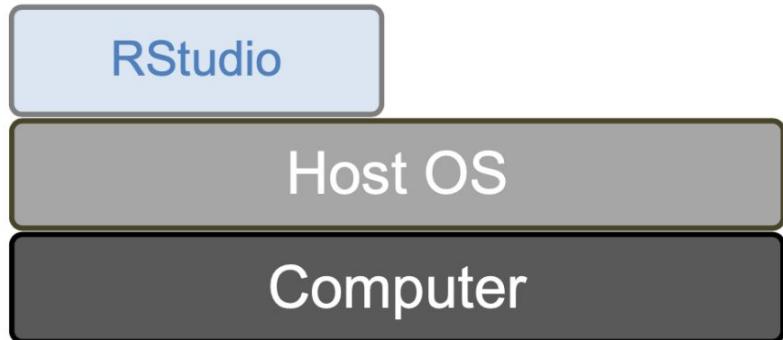
### Unix-based

A terminal window on a Unix-based system (Ubuntu 18.04) showing the command to install RStudio from a deb package. The output of the command `sudo dpkg -i ~/Downloads/rstudio-1.2.5001-amd64.deb` is displayed, showing the progress of the package build and dependency resolution. The terminal ends with the message "Reading state information... done".



We started with a computer using a specific OS...





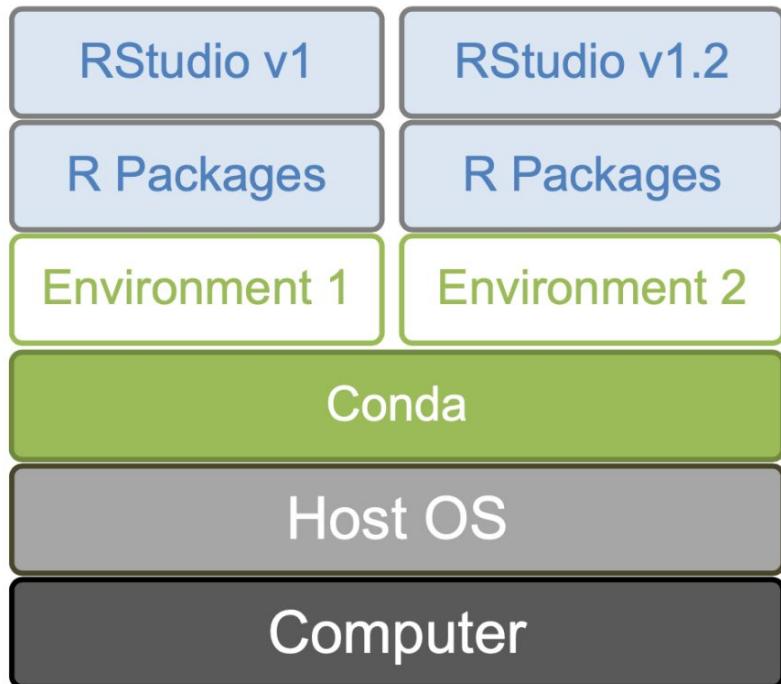
We started with a computer using a specific OS...  
And inside this environment, we installed a new application.



Usually dependencies of different applications don't interfere.  
But what if we want to test the latest version of our favourite tool?  
There might be conflicts...

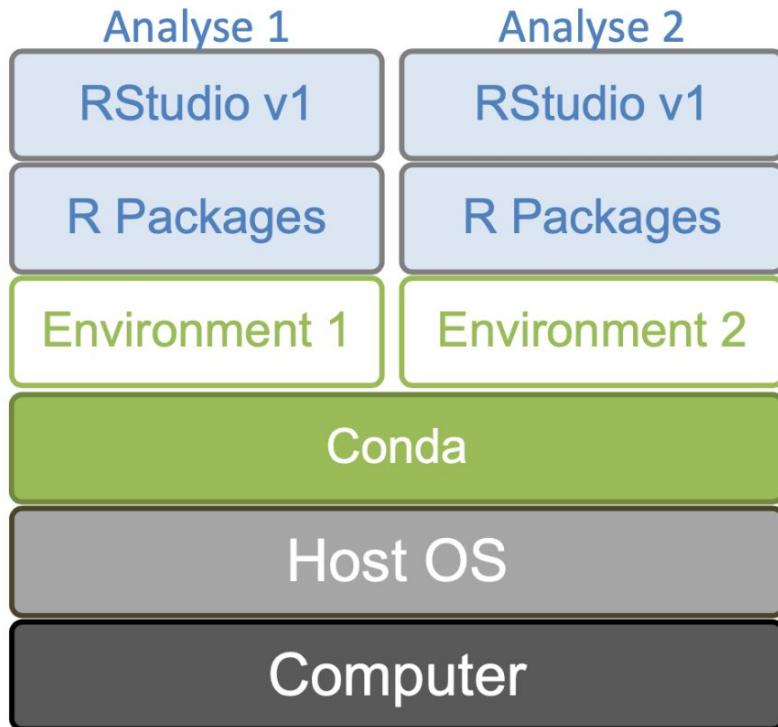


Usually dependencies of different applications don't interfere.  
But what if we want to test the latest version of our favourite tool?  
There might be conflicts...

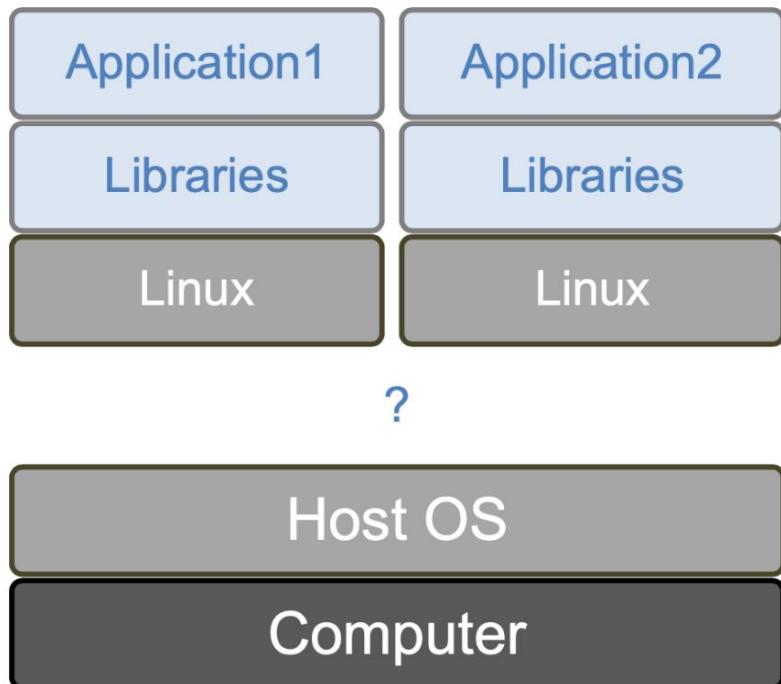


Idea : create separated environments  
for each application.

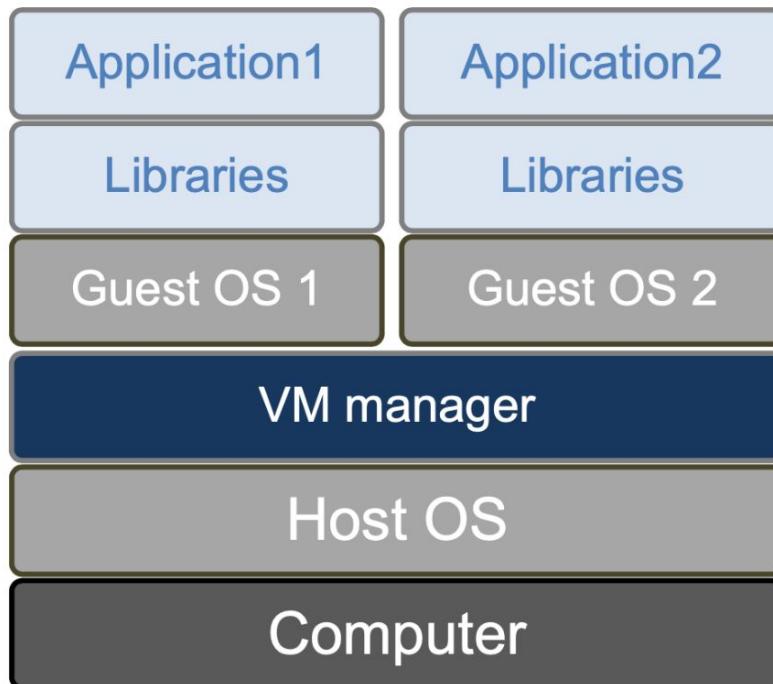
**CONDA**



Idea : create separated environments  
for each application.  
More versatile: create a new  
environment per analysis.



But what if we want to install a software from a different OS?

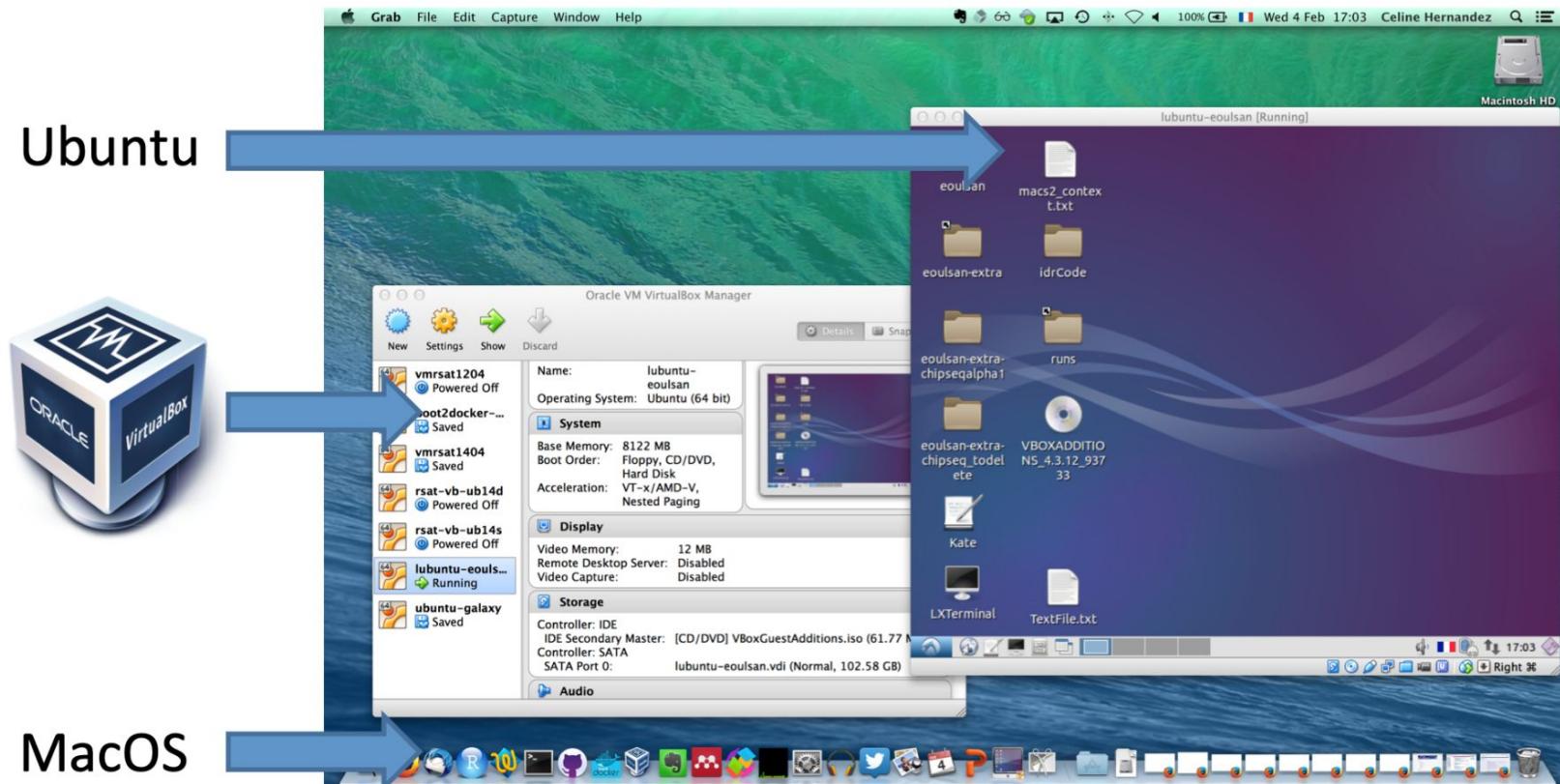


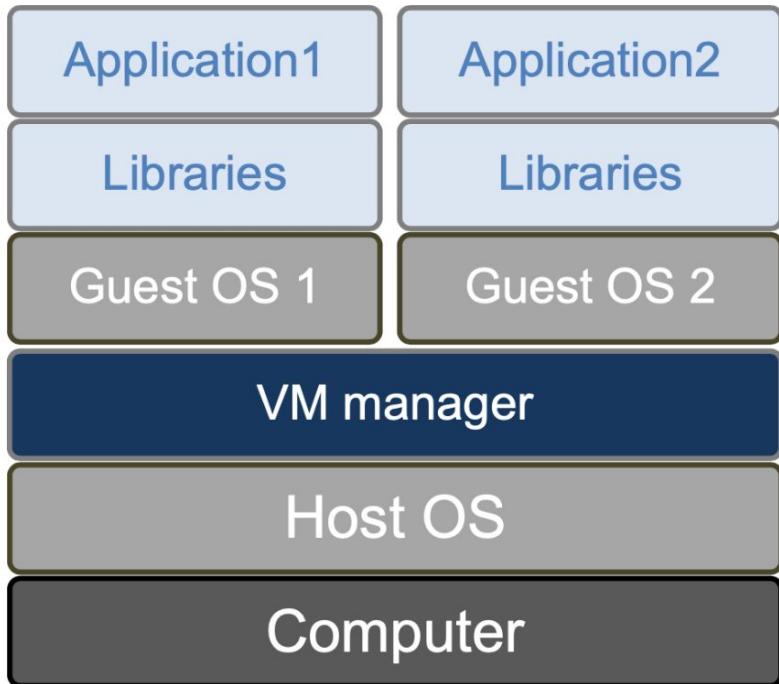
Idea: use virtual machines

Pros:

- Each application gets a completely different and independent environment
- Virtual machines can be transferred to another computer (using the same manager)

# Encapsulation : hardware virtualization





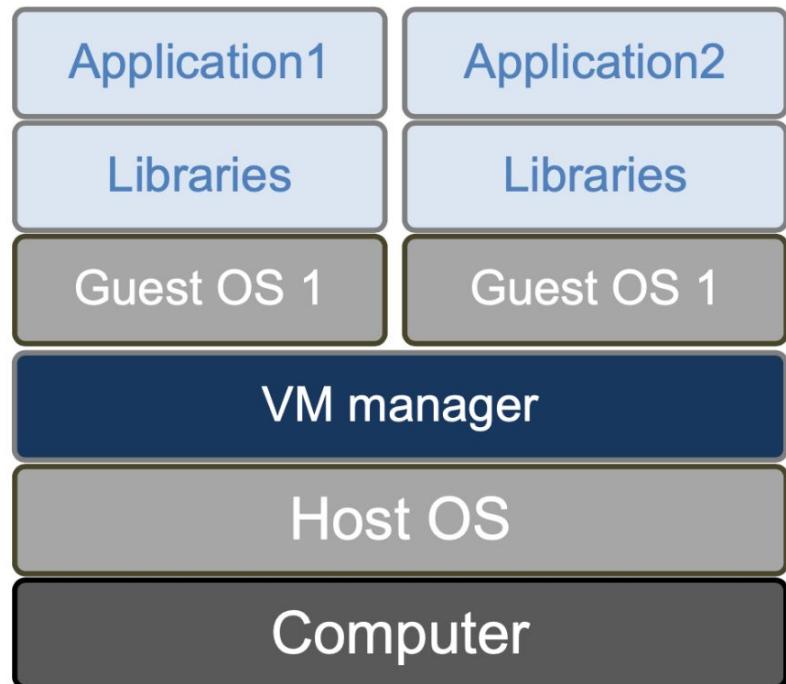
Idea: use virtual machines

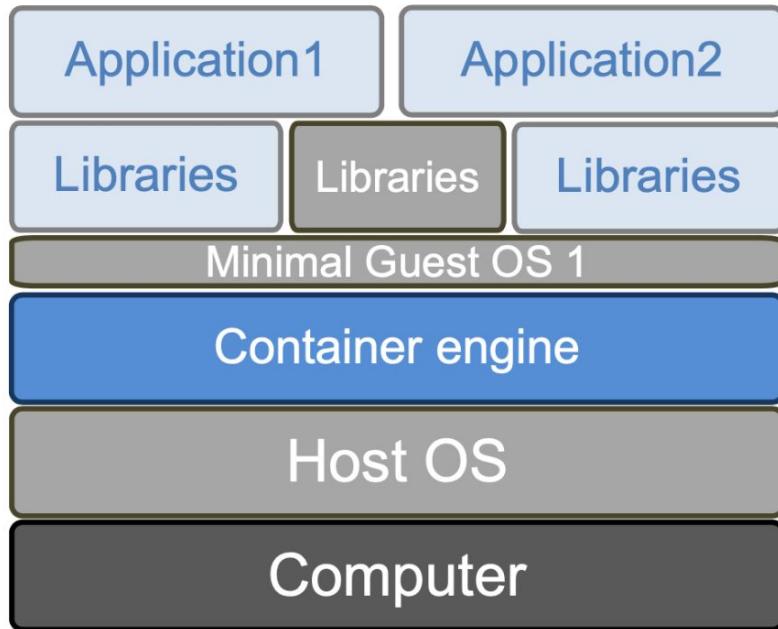
Pros: transferable independent environments

Cons:

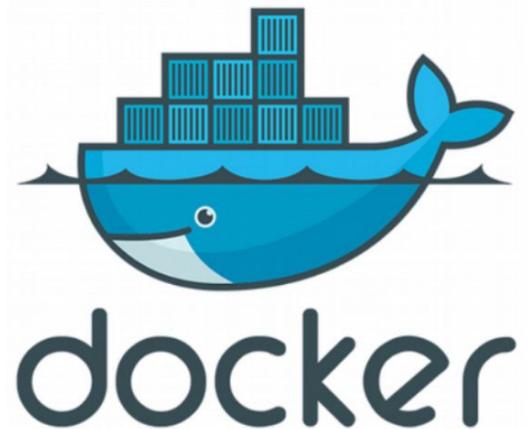
- Redundancy between VMs
- Heavy to set up
- No automation

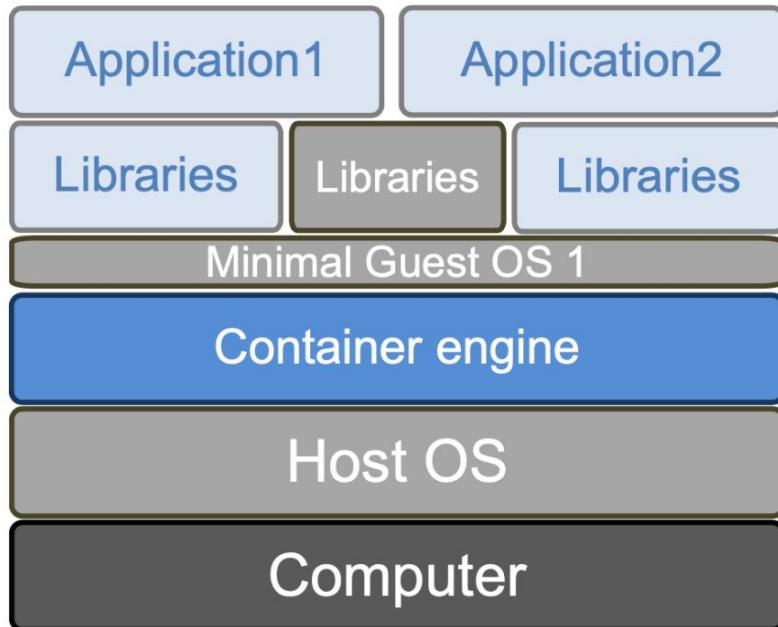
# Encapsulation : OS virtualization





Idea: "trick" applications into believing that they are in a different OS than the host's  
Avoid redundancy.

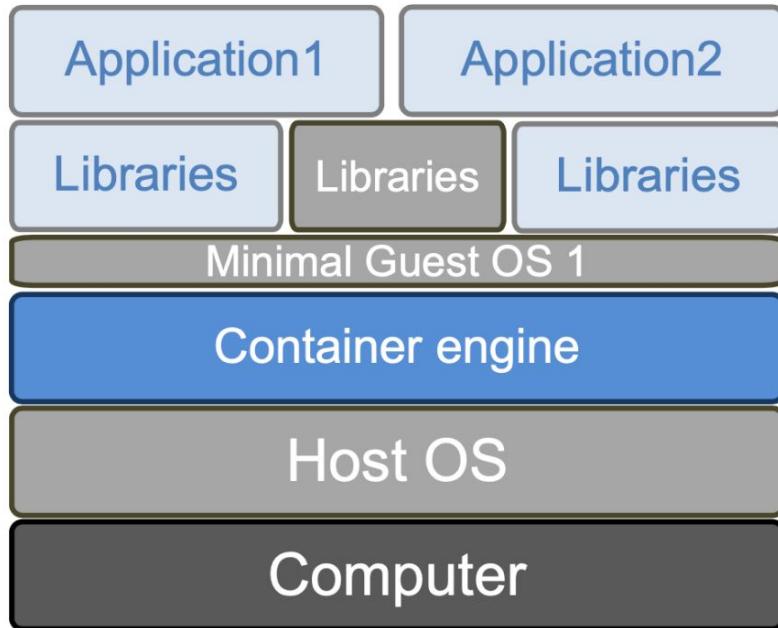




## OS virtualisation vs hardware virtualisation

Pros:

- Speed
  - ▶ Installation is faster
  - ▶ No boot time
- Lightweight
  - ▶ Minimal base OS
  - ▶ Minimal libraries and application set
- Easy sharing of applications



## Cons:

- Singularity to use images on a cluster
- Changes of policies of the Docker company



## Update of the Docker Image retention policy (13/08/2020)

### What is a container image retention limit and how does it affect my account?

Image retention is based on the activity of each individual image stored within a user account. If an image has not either been pulled or pushed in the amount of time specified in your subscription plan, the image will be tagged “inactive.” Any images that are tagged as “inactive” will be scheduled for deletion. Only accounts that are on the **Free** individual or organization plans will be subject to image retention limits. A new dashboard will also be available in Docker Hub that offers the ability to view the status of all of your container images.

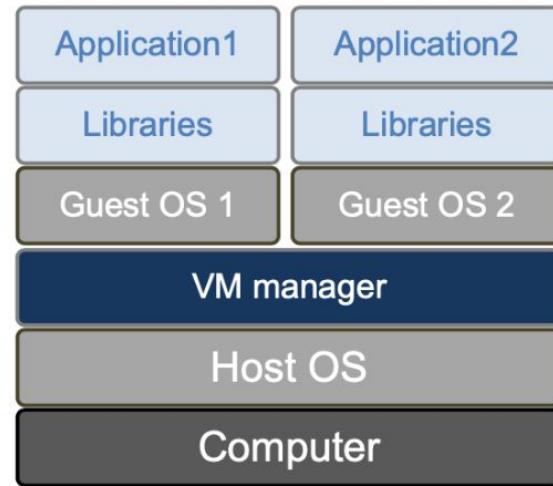
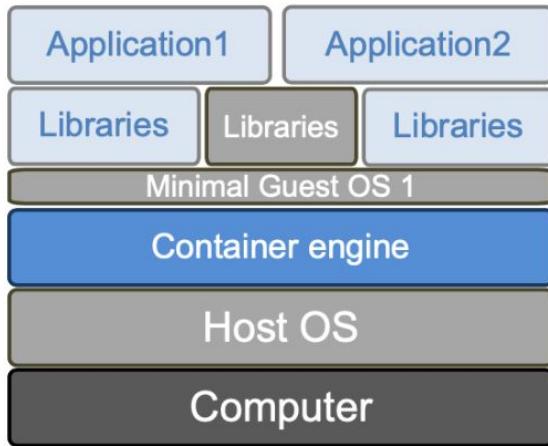
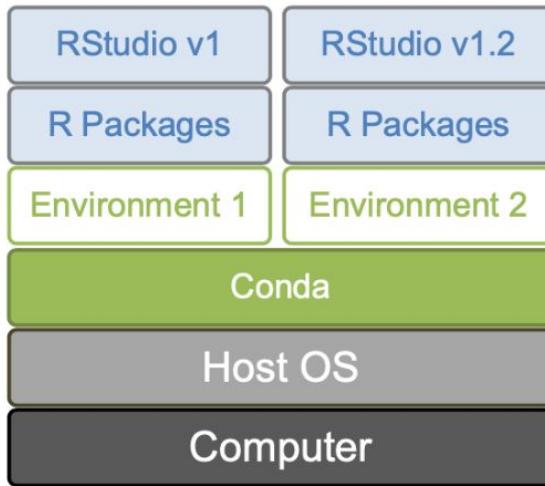
### What are the new container image retention limits?

Docker is introducing a container image retention policy which will be enforced starting November 1, 2020. The container image retention policy will apply to the following plans:

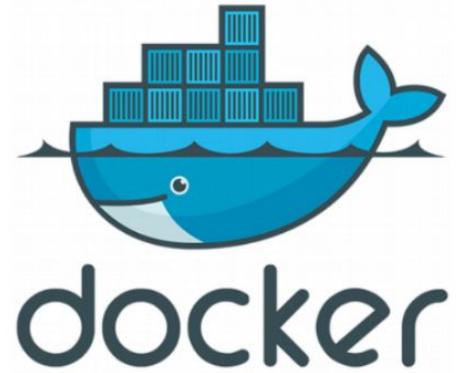
- Free plans will have a 6 month image retention limit
- Pro and Team plans will have unlimited image retention

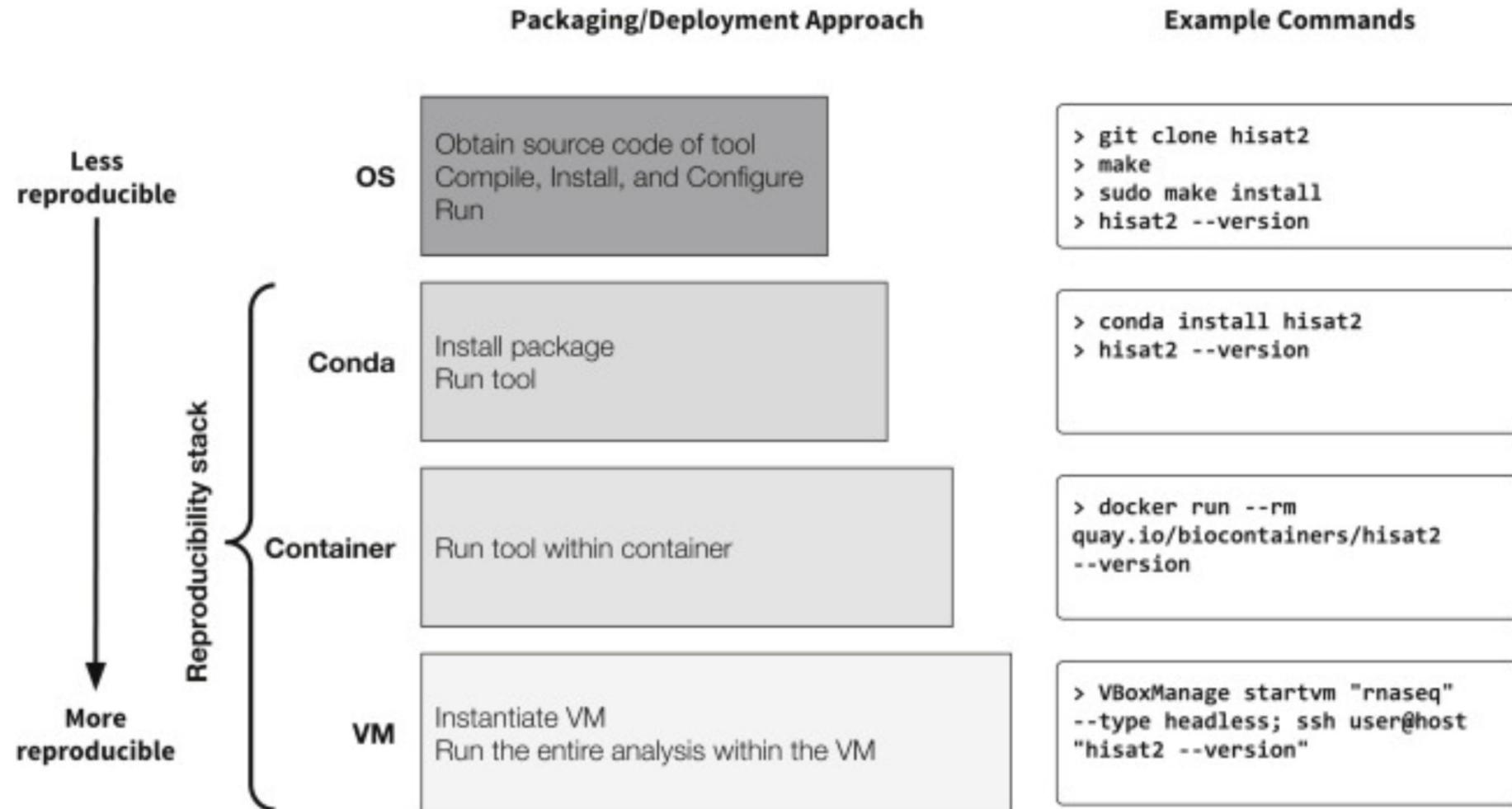
<https://www.docker.com/pricing/retentionfaq>

# Encapsulation



CONDA





Practical Computational Reproducibility in the Life Sciences - Björn  
Grüning et al (2018)





# Docker





Docker is not very “old”

- First commit January 2013
- First version March 2013
- Version 1.0 in June 2014

But its adoption was fast

- Officially packaged in Ubuntu since 2014 (v14.04)



## Image



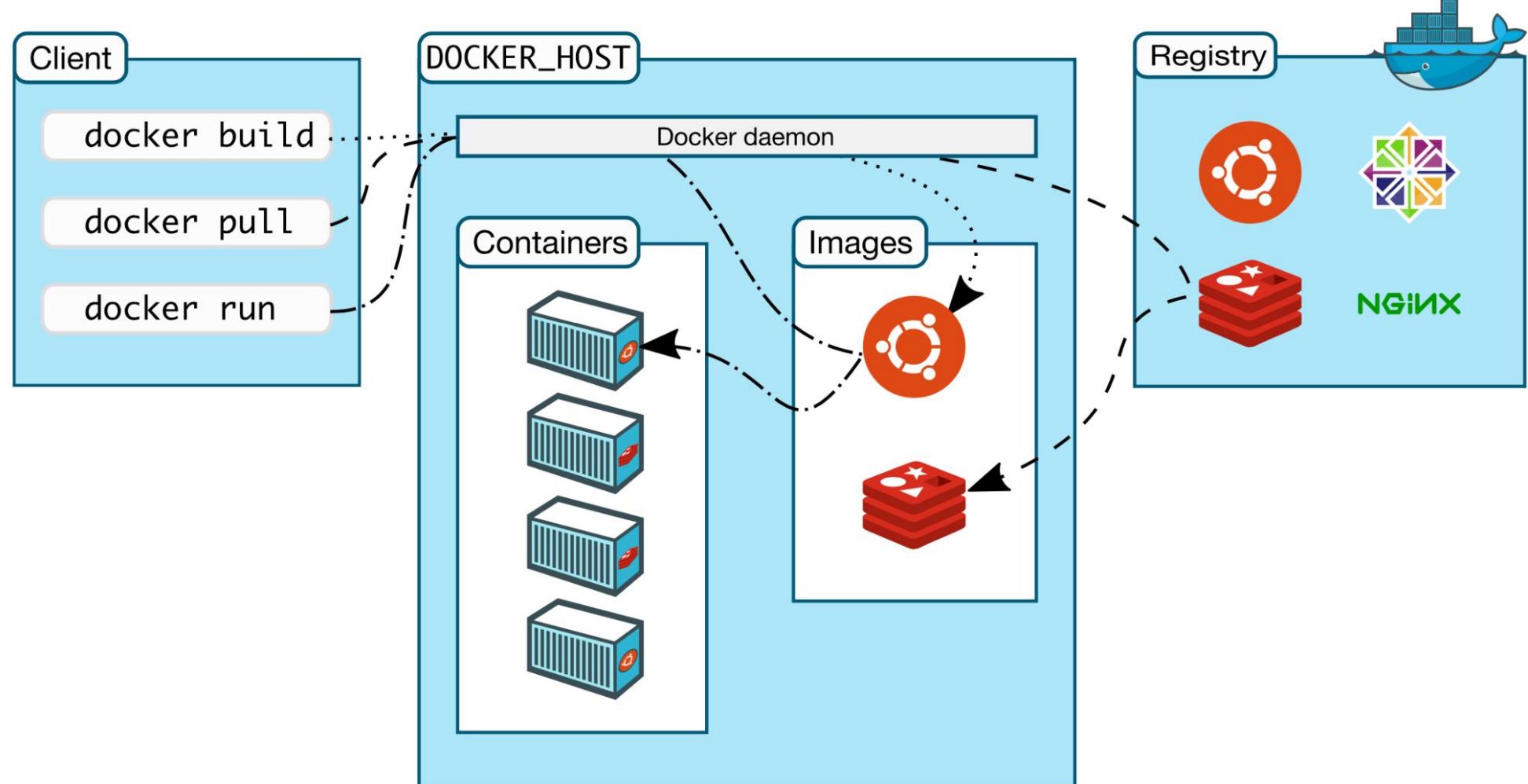
## Container



- Set of libraries and functions
- Fixed. Cannot be modified
- Can be stored/shared online
- Can be automatically built

- "Active image"
- Can be modified (interactive)
- Can be turned into an image
- One image, many containers

# What is Docker?



(<https://docs.docker.com/get-started/overview/>)

# What is Docker?



The screenshot shows the Docker Hub interface. At the top, there's a navigation bar with a search bar, a Docker logo, and links for 'Explore', 'Help', 'Sign up', and 'Sign in'. A banner at the top of the main content area says 'Docker Store is the new place to discover public Docker content. Check it out →'. Below this, the heading 'Explore Official Repositories' is displayed. The main content is a list of official Docker repositories, each represented by a card:

Repository	Owner	Stars	Pulls	Actions
nginx	NGINX official	5.3K STARS	10M+ PULLS	<a href="#">DETAILS</a>
redis	redis official	3.4K STARS	10M+ PULLS	<a href="#">DETAILS</a>
busybox	Buildroot official	924 STARS	10M+ PULLS	<a href="#">DETAILS</a>
ubuntu	ubuntu official	5.5K STARS	10M+ PULLS	<a href="#">DETAILS</a>
registry	docker official	1.3K STARS	10M+ PULLS	<a href="#">DETAILS</a>

(<https://hub.docker.com/>)

# What is Docker?



## Usermade images (1/2)

The screenshot shows the Docker Hub user profile for 'genomicpariscentre'. The profile picture is a placeholder user icon. The profile name is 'genomicpariscentre' and the organization name is 'Genomic Paris Centre'. It shows the location as 'Paris', the website as 'http://genomique.biologie.ens.fr/', and the joining date as 'Joined June 2014'. Below the profile information, there is a list of eight Docker images:

Image Name	Status	Stars	Pulls	Action
genomicpariscentre/star	public   automated build	1 STARS	1.2K PULLS	DETAILS
genomicpariscentre/bcl2fastq2	public   automated build	0 STARS	1.2K PULLS	DETAILS
genomicpariscentre/blast2	public   automated build	0 STARS	765 PULLS	DETAILS
genomicpariscentre/bcbio-nextgen	public   automated build	0 STARS	451 PULLS	DETAILS
genomicpariscentre/fastqc	public   automated build	0 STARS	404 PULLS	DETAILS
genomicpariscentre/bowtie2	public   automated build	0 STARS	308 PULLS	DETAILS
genomicpariscentre/samtools	public   automated build	0 STARS	304 PULLS	DETAILS
genomicpariscentre/eouslan	public   automated build	2 STARS	231 PULLS	DETAILS

(<https://hub.docker.com/u/genomicpariscentre/>)



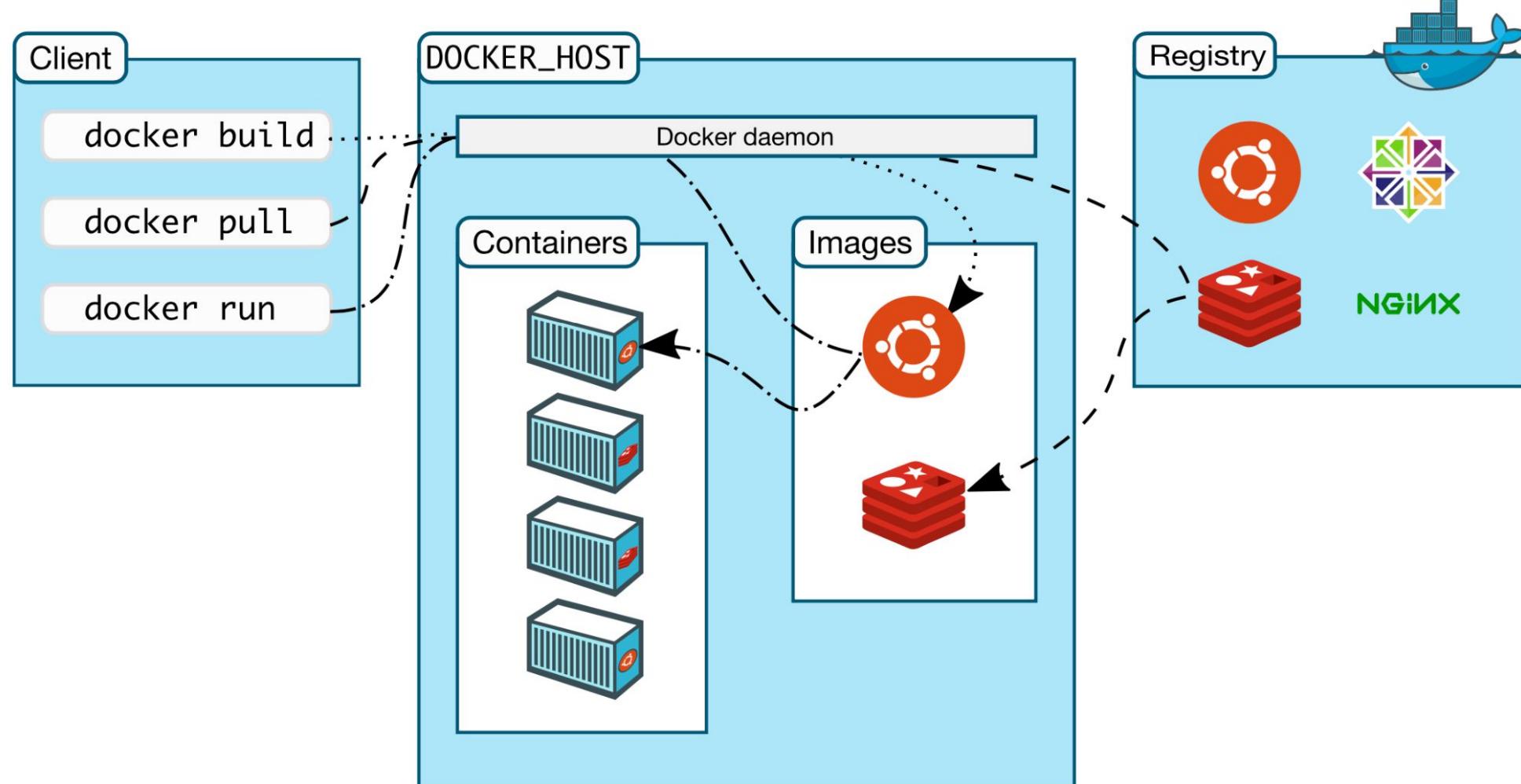
## Usermade images (2/2)

Be critical!

The screenshot shows the Docker Hub interface for the repository `genomicpariscentre/samtools`. The page title is "PUBLIC | AUTOMATED BUILD". The repository name is displayed prominently with a star icon. Below it, the text "Last pushed: 2 years ago" is shown. The interface includes tabs for "Repo Info", "Tags", "Dockerfile", and "Build Details", with "Repo Info" being the active tab. The "Short Description" field contains the text: "Samtools is a processor of sequence alignments fot SAM and BAM formats". The "Docker Pull Command" field contains the command: `docker pull genomicpariscentre/samtools`. The "Owner" field shows the user `genomicpariscentre`. The "Source Repository" field links to `GenomicParisCentre/dockerfiles`.

(<https://hub.docker.com/r/genomicpariscentre/samtools/>)

# What is Docker?



(<https://docs.docker.com/get-started/overview/>)



## Other commands :

- docker images : list images available locally
- docker ps : status of containers
- docker rm : delete a container
- docker rmi : delete an image
- ...

(More details during the practical session.)

