FAIR_bioinfo : Open Science and FAIR principles in a bioinformatics project

How to make a bioinformatics project more reproducible

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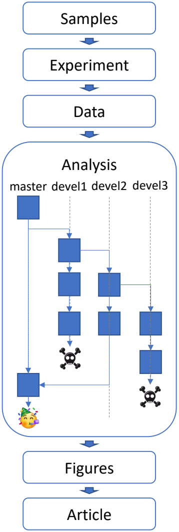
June 2021

Introduction

A (not-so-uncommon) nightmare



Samples

Experiment

Data

Analysis

master devel1 devel2 devel3

Figures

Article

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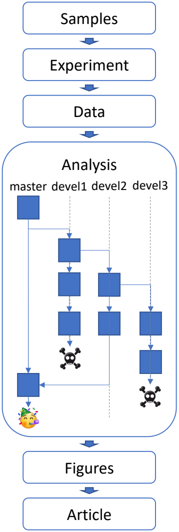

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Submit to a journal

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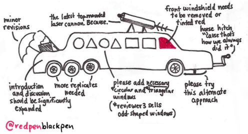

Reviewer 3

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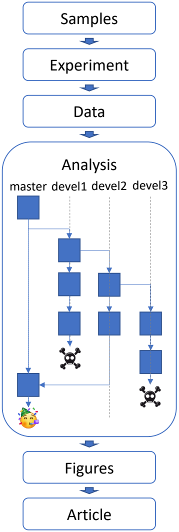

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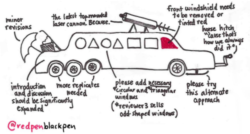

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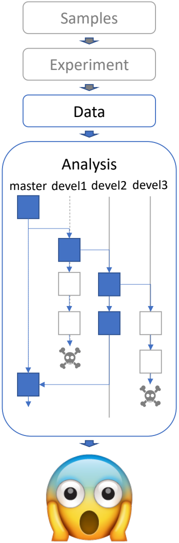

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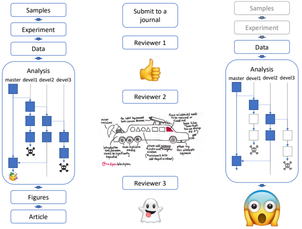

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What changed?

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

Different levels of encapsulation

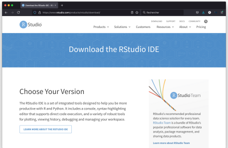
Goal : capture the system environment of applications (OS, packages, libraries,. . .) to control their execution.

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

Encapsulation

Let’s say we want to install RStudio…

Install Rstudio ?



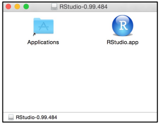
Download the RStudio IDE

Choose Your Version

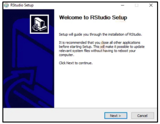
The RStudio IDE is a set of integrated tools designed to help you be more productive with R and Python. It includes a console, syntax-highlighting editor that supports direct code execution, and a variety of robust tools for plotting, viewing history, debugging and managing your workspace.

RStudio’s recommended professional data science solution for every team. RStudio Team is a bundle of RStudio’s popular professional software for data analysis, package management, and sharing data products.

MacOS



Windows



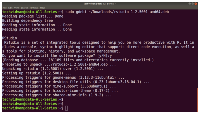
Welcome to RStudio Setup

Setup will guide you through the installation of RStudio.

It is recommended that you close all other applications before starting Setup. This will make it possible to update relevant system files without having to reboot your computer.

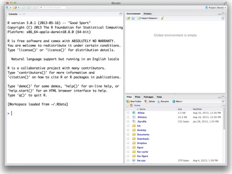
Click Next to continue.

Unix-based



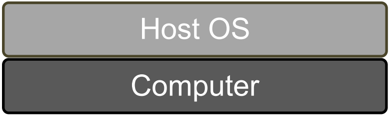
```
techvidvan@data-All-Series:~$ sudo gdebi ~/Downloads/rstudio-1.2.5001-amd64.deb
Reading package lists... Done
Building dependency tree
Reading state information... Done
Reading state information... Done

RStudio
 RStudio is a set of integrated tools designed to help you be more productive with R. It in
cludes a console, syntax-highlighting editor that supports direct code execution, as well a
s tools for plotting, history, and workspace management.
Do you want to install the software package? [y/N]:y
(Reading database ... 181189 files and directories currently installed.)
Preparing to unpack .../rstudio-1.2.5001-amd64.deb ...
Unpacking rstudio (1.2.5001) over (1.2.5001) ...
Setting up rstudio (1.2.5001) ...
Processing triggers for gnome-menus (3.13.3-1ubuntu1) ...
Processing triggers for desktop-file-utils (0.23-1ubuntu3.18.04.1) ...
Processing triggers for mime-support (3.60ubuntu1) ...
Processing triggers for hicolor-icon-theme (0.17-2) ...
Processing triggers for shared-mime-info (1.9-2) ...
techvidvan@data-All-Series:~$
techvidvan@data-All-Series:~$
techvidvan@data-All-Series:~$ 
```

Use Rstudio



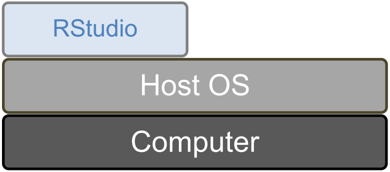
```
R version 3.0.1 (2013-05-16) -- "Good Sport"
Copyright (C) 2013 The R Foundation for Statistical Computing
Platform: x86_64-apple-darwin10.8.0 (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

[Workspace loaded from ~/.RData]

> 
```

Encapsulation



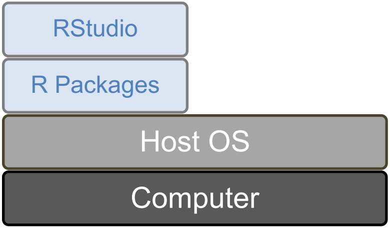
We started with a computer using a specific OS...

Encapsulation



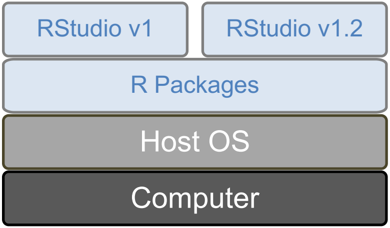
We started with a computer using a specific OS...
And inside this environment, we installed a new application.

Encapsulation



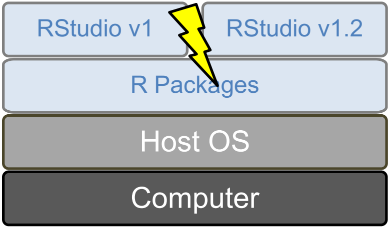
We started with a computer using a specific OS...
And inside this environment, we installed a new application.
Applications rely on dependencies, e.g. external libraries.

Encapsulation



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. . .

Encapsulation



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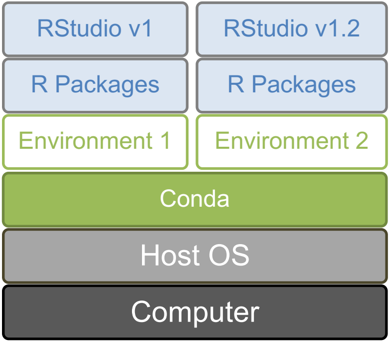
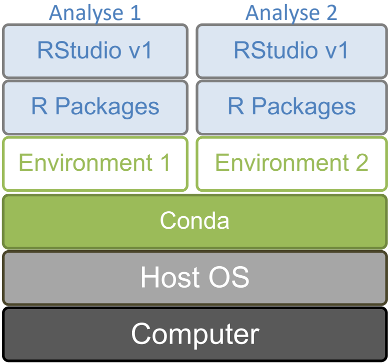
There might be conflicts. . .

Encapsulation : managing environments



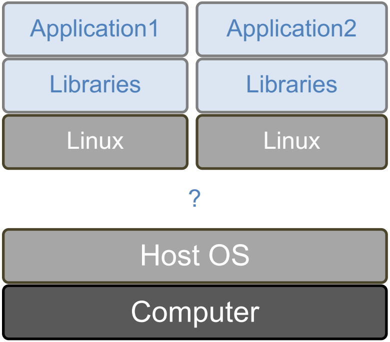
Idea : create separated environments for each application.

Encapsulation : managing environments



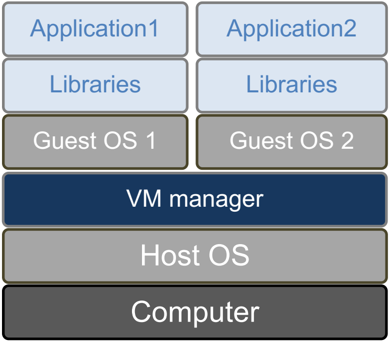
Idea : create separated environments for each application.
More versatile: create a new environment per analysis.

Encapsulation : hardware virtualisation



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

Encapsulation : hardware virtualisation

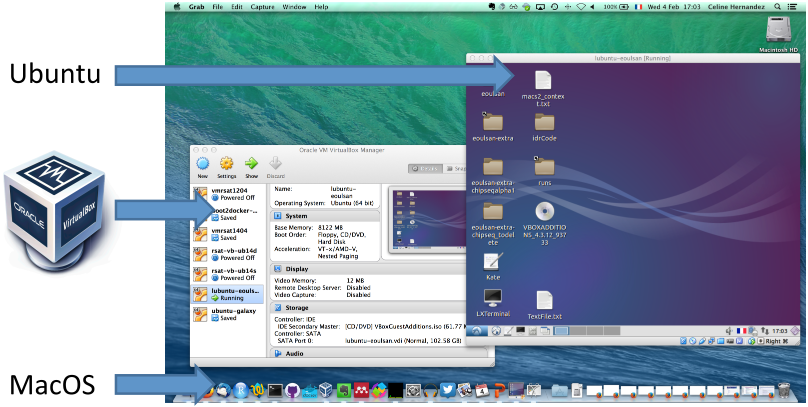


Idea: use virtual machines

Pros:

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

Encapsulation : hardware virtualisation


Ubuntu

MacOS

vmrsat1204 Powered Off
boot2docker-... Saved
vmrsat1404 Saved
rsat-vb-ub14d Powered Off
rsat-vb-ub14s Powered Off
lubuntu-eouls... Running
ubuntu-galaxy Saved

Name: lubuntu-eoulsan
Operating System: Ubuntu (64 bit)

System

Base Memory: 8122 MB
Boot Order: Floppy, CD/DVD, Hard Disk
Acceleration: VT-x/AMD-V, Nested Paging

Display

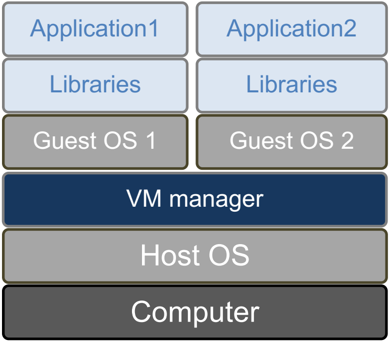
Video Memory: 12 MB
Remote Desktop Server: Disabled
Video Capture: Disabled

Storage

Controller: IDE
IDE Secondary Master: [CD/DVD] VBoxGuestAdditions.iso (61.77
Controller: SATA
SATA Port 0: lubuntu-eoulsan.vdi (Normal, 102.58 GB)

Audio

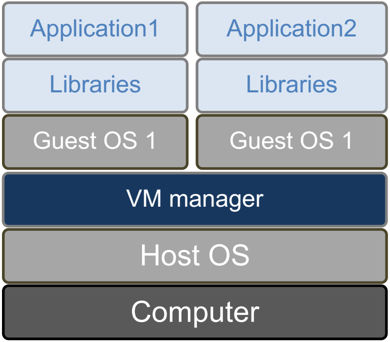
Encapsulation : hardware virtualisation



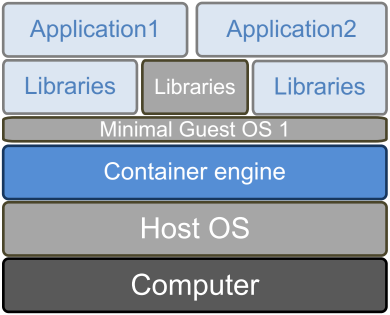
Idea: use virtual machines
Pros: transferable independent environments
Cons:

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

Encapsulation : OS virtualisation



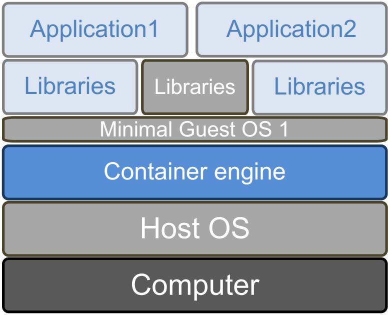
Encapsulation : OS virtualisation



Application1
Application2
Libraries
Libraries
Libraries
Minimal Guest OS 1
Container engine
Host OS
Computer

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

Encapsulation : OS virtualisation

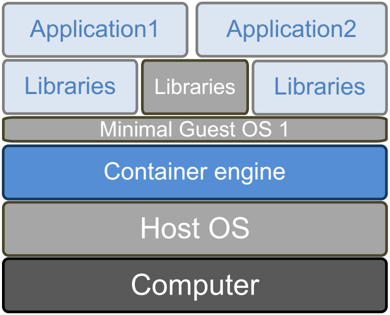


OS virtualisation vs hardware virtualisation

Pros:

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

Encapsulation : OS virtualisation

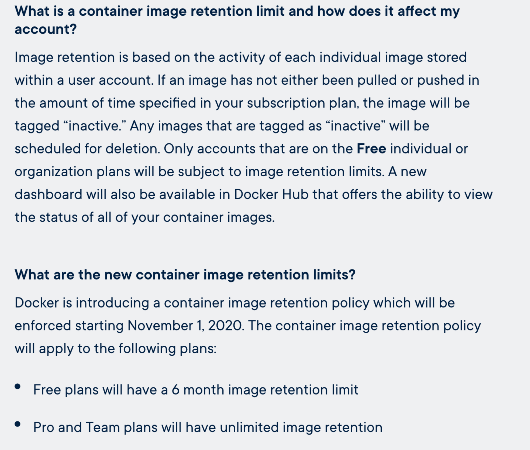


Cons:

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

Docker policy

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.

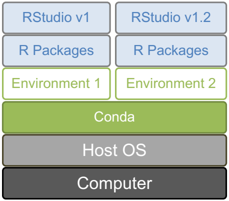
What are the new container image retention limits?

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



RStudio v1 | RStudio v1.2

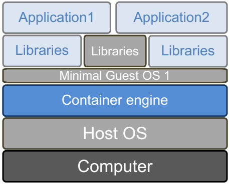
R Packages | R Packages

Environment 1 | Environment 2

Conda

Host OS

Computer



Application1 | Application2

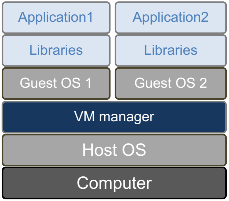
Libraries | Libraries | Libraries

Minimal Guest OS 1

Container engine

Host OS

Computer



Application1 | Application2

Libraries | Libraries

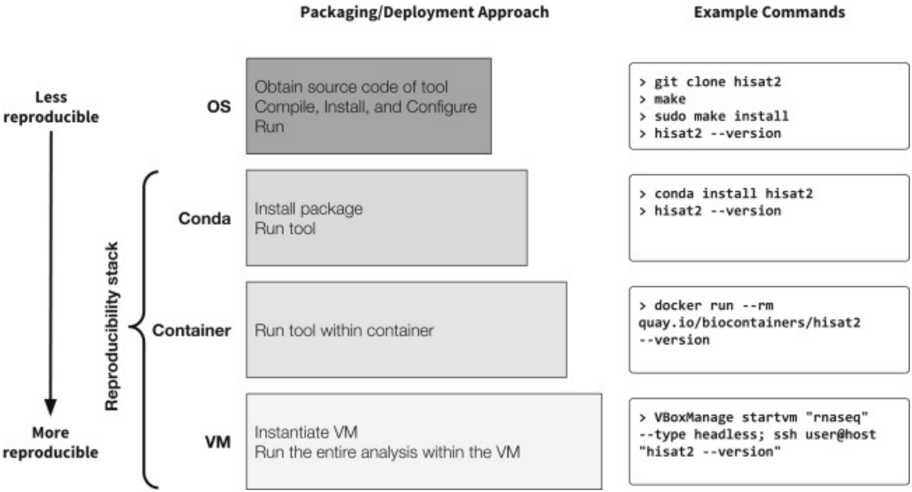
Guest OS 1 | Guest OS 2

VM manager

Host OS

Computer

Encapsulation and reproducibility stack



OS

Obtain source code of tool
Compile, Install, and Configure
Run

```
> git clone hisat2
> make
> sudo make install
> hisat2 --version
```

Conda

Install package
Run tool

```
> conda install hisat2
> hisat2 --version
```

Container

Run tool within container

```
> docker run --rm
quay.io/biocontainers/hisat2
--version
```

VM

Instantiate VM
Run the entire analysis within the VM

```
> VBoxManage startvm "rnaseq"
--type headless; ssh user@host
"hisat2 --version"
```

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

Conda

CONDA: an environment manager

Conda definitions

- Environment: a set of packages/tools in a directory (added to our PATH)
- Conda: an open source package + a general-purpose environment management system (installation, execution, upgrade). For any programming language, multi-platform (Windows, MacOS, Linux).
- Conda package: a compressed tarball of a tool

Why using an environment manager?

- avoid compilation and dependencies problems: an environment manager will take care of everything!
- have several environments in parallel each with their own set of tools
- useful when cross-tools dependencies are incompatible with each other

CONDA: Access

Conda distribution

- Anaconda: a data science platform, comes with a lot of packages
- Miniconda: come without installed packages

Anconda cloud, the "conda hub"

- Anaconda cloud (private company) relies on the community of developers, concerns many domains (Machine Learning, Data Visualization, Dashboarding-web, Image Processing, Natural Language Processing, etc)
- Anaconda cloud: made up of channels/owners. Each channels contains one or more conda packages
- be careful when downloading any packages from an untrusted source, always inspect before installation

CONDA About channels

Some conda channels

- `default`
- `conda-forge`: many popular python packages (analogous to PyPI but with a unified, automated build infrastructure and more peer review of recipes)
- `bioconda`: bioinformaticians' contributions
- private

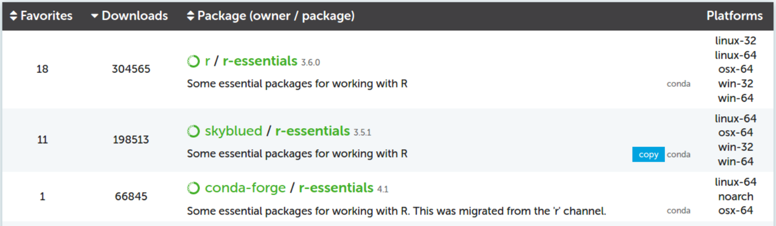
Channels list order

- when different channels have the same package ⇒ collisions
- collisions resolved following the order of your channels list ⇒ put supplemental channels at the bottom of your channel list

CONDA R, mamba

Conda and R

The R interpreter is included in the `r-essentials` package (200 r packages). Add `r-` before the regular r package name (eg. `r-ggplot2`)



Favorites	Downloads	Package (owner / package)	Platforms
18	304565	r / **r-essentials** 3.6.0 Some essential packages for working with R conda	linux-32 linux-64 osx-64 win-32 win-64
11	198513	skyblued / **r-essentials** 3.5.1 Some essential packages for working with R copy conda	linux-64 osx-64 win-32 win-64
1	66845	conda-forge / **r-essentials** 4.1 Some essential packages for working with R. This was migrated from the 'r' channel. conda	linux-64 noarch osx-64

Mamba

A fast drop-in alternative to conda, using libsolv for dependency resolution

```
conda install -c conda-forge mamba
```

Next, replace `conda` by `mamba` to use it

CONDA command

simple commands

```
conda create env -n myenv # creation of a conda environment
conda info --envs # list environments (* for the active one)
conda activate myenv # active the myenv environment
conda list # list packages (only in an active environment)
conda install package # installation of a tool/package
conda remove package # suppress the tool from the environment
conda env remove -n myenv # suppress the myenv environment
conda deactivate # inactivate the environment
```

miniconda3

With the miniconda3 distribution and by default, environments are installed in a `miniconda3/envs/` repository

CONDA 2 modes

interactive

- create an environment
- activate the environment
- install some conda packages

configuration file

- list all conda packages in a configuration file (`yaml` or `json` format)
- create the environment based on the configuration file (option `-f`)
- activate the environment

reproducibility

- good practice: use a configuration file
- specify a precise version of a package:
  `<channel>::<package>=<version>`

Conda Exercise

Conda setup

How to access conda?

- Conda is so used that it could even be installed by default to your machine. To test this: `conda --version`
- if not, may install it or got it by a docker image:

```
docker run -i -t -v ${PWD}:/data continuumio/miniconda3
```

- already activated on the IFB cluster (otherwise with module: `module load conda`)

How to access tools?

Manage Conda environment

1. create the working environment:

```
conda create env -n myenv
```

2. activate it:

```
conda activate myenv
```

3. if not yet done, install packages (specify the channel):

```
conda install -c bioconda bowtie2
```

4. work with the tools
5. quite the environment:

```
conda deactivate
```

Install snakemake with conda

Objective

Create a conda configuration file to install the snakemake tool.

Hint

- Search its channel in the Anaconda cloud web pages
- the "minimal" environment is sufficient

Install snakemake with conda

condaEnvSmk.yml

```
channels:
  - conda-forge
  - bioconda
  - main
dependencies:
  - snakemake-minimal=6.5.0
```

run

```
conda env create -n condaEnvSmk -f condaEnvSmk.yml
conda activate condaEnvSmk
snakemake --version
```

Docker

What is 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)

What is Docker?

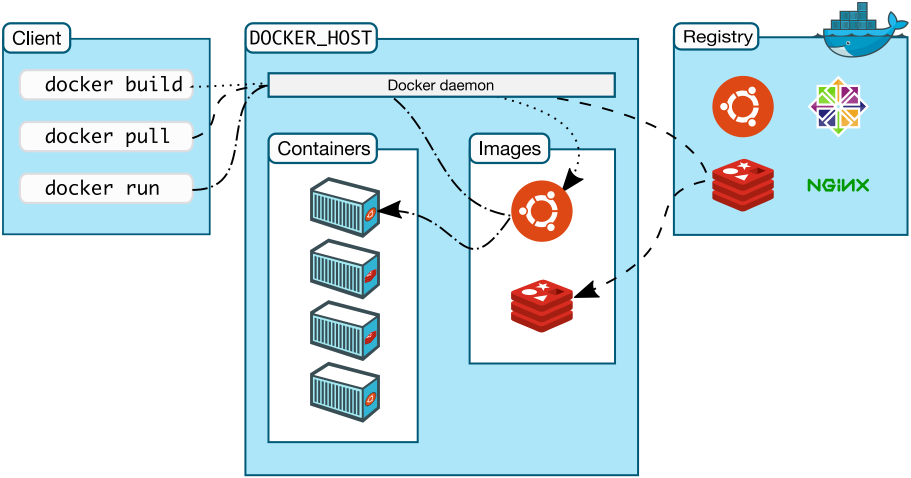
Image

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

Container

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

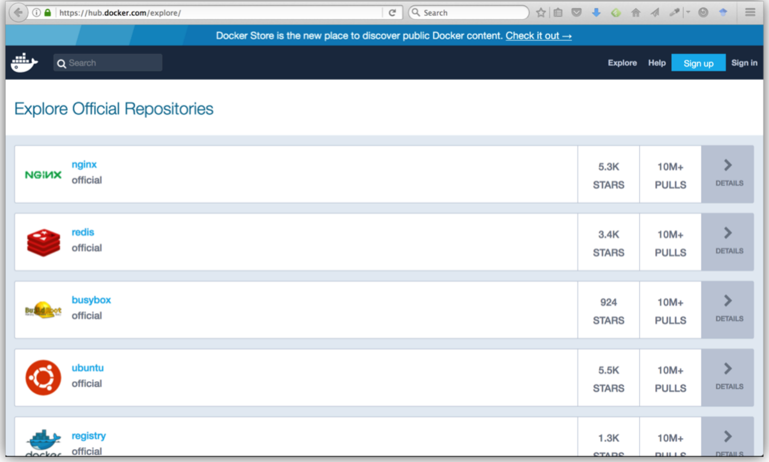
What is Docker?



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

What is Docker?

DockerHub



https://hub.docker.com/explore/

Docker Store is the new place to discover public Docker content. Check it out →

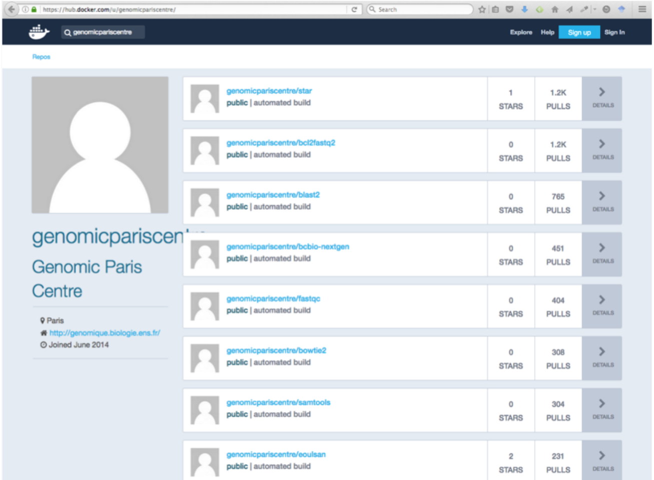
Explore Official Repositories

nginx official	5.3K STARS	10M+ PULLS	DETAILS
redis official	3.4K STARS	10M+ PULLS	DETAILS
busybox official	924 STARS	10M+ PULLS	DETAILS
ubuntu official	5.5K STARS	10M+ PULLS	DETAILS
registry official	1.3K STARS	10M+ PULLS	DETAILS

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

What is Docker?

Usermade images (1/2)



https://hub.docker.com/u/genomicpariscentre/

genomicpariscentre

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Repos

genomicpariscen

Genomic Paris Centre

Paris

http://genomique.biologie.ens.fr/

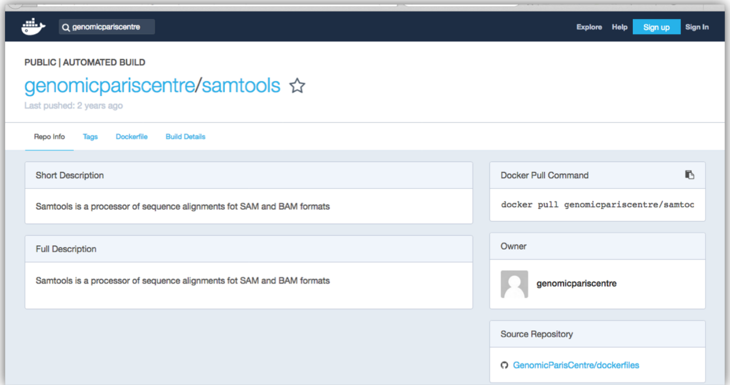
Joined June 2014

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/eoulsan	**public** | automated build	2 STARS	231 PULLS	DETAILS

(urlhttps://hub.docker.com/u/genomicpariscentre/)

What is Docker?

Usermade images (2/2)
Be critical!



PUBLIC | AUTOMATED BUILD

genomicpariscentre/samtools ☆

Last pushed: 2 years ago

Short Description

Samtools is a processor of sequence alignments fot SAM and BAM formats

Full Description

Samtools is a processor of sequence alignments fot SAM and BAM formats

Docker Pull Command

```
docker pull genomicpariscentre/samtoc
```

Owner

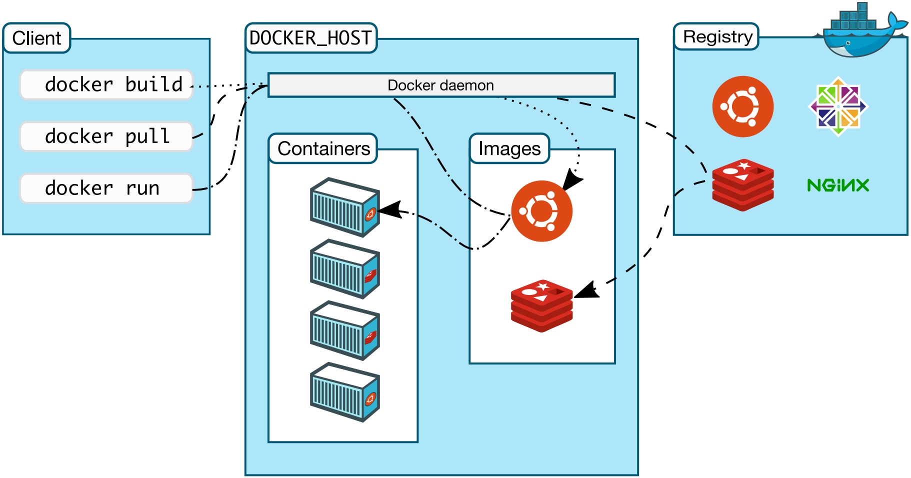
genomicpariscentre

Source Repository

GenomicParisCentre/dockerfiles

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

What is Docker?



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

What is Docker?

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.)

Practical session

Savoir FAIRe

- (Installation de Docker)
- 1. Use a pre-defined image available on the DockerHub
- 2. Adapt an image to your needs
- 3. Build an image with a Dockerfile

Practical session : Docker and FastQC. See companion document.