Docker and containerization

- an introduction -

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About me

BSc in Computer Science with a thesis on High Performance Computing at SISSA

MSc in computational physics with a thesis on Big Data at CERN

CERN research fellow working on new computing and data analysis methodologies

Then, 5 years in startups.

- Core team member of an IoT energy metering and analytics startup,
- Joined Entrepreneur First, Europe's best deep tech startup accelerator
- ..and co-founded Sharpsense (analysed the Genoa Morandi Bridge data after the collapse)

Meanwhile: always kept the link with academia.

- Lectured on Big Data for scientific computing at the Master In High Performance Computing (SISSA and UN's ICTP),
- Worked on data processing pipelines for EUMETSAT,
- Held seminars about "Modern Software Development" in universities.

Now: back into research (INAF).

A note on the startup world

Tech startups

Use new technologies

→ R&D is not the core business

Examples:

- Facebook
- AirBnB
- Amazon
- Twitter
- Uber
- ...and all the "yet another App".

Deep Tech startups

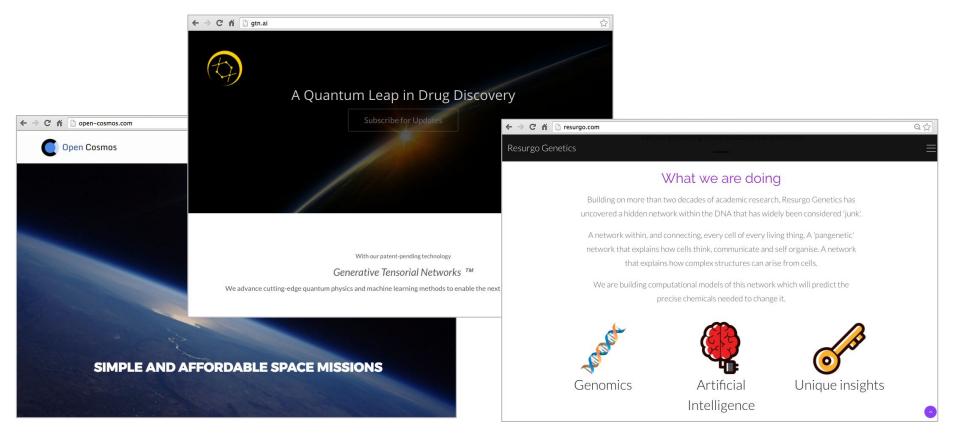
Develop new technologies

→ R&D is the core business

Examples:

- Google
- Deep Mind
- Tesla
- SpaceX
- Human Longevity
- ..and all the university spin-offs.

A note on the startup world



A note on the startup world

- 1) Startups are extremely resource-constrained
- 2) Time is a precious asset
- 3) Deep tech startups have complex codebases

1 + 2 + 3 = You really don't want to fall in a "dependency hell"

The "dependency hell" problem

Mike wants to install a new software.

Mike cannot find a precompiled version that works with his OS and/or libraries.

Mike ask/Google for help and get some basic instructions - like "compile it".

Mike starts downloading all the development environment, and soon realizes that he needs to upgrade (or downgrade!) some parts of his main Operating Systems.

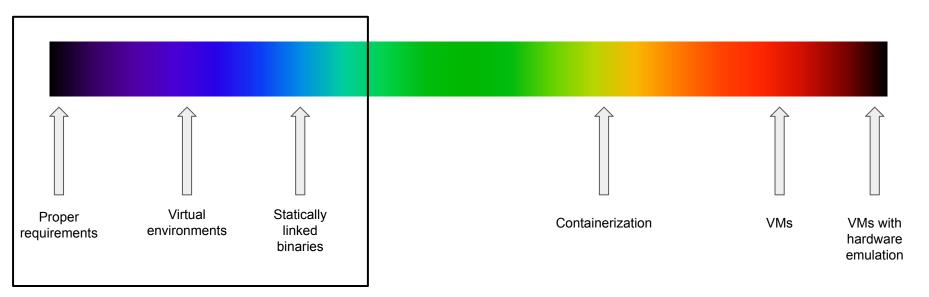
During this process, something goes wrong.

Mikes spends an afternoon fixing his own OS, and all the next day in trying to compile the software. Which at the end turns out not to do what he wanted.

The "dependency hell" problem: solutions spectrum



The "dependency hell" problem: solutions spectrum



Proper requirements

- Carefully keep track of what libraries/OS features are used in development and report them on the documentation, for each release.
- Prone to human error we stop here.

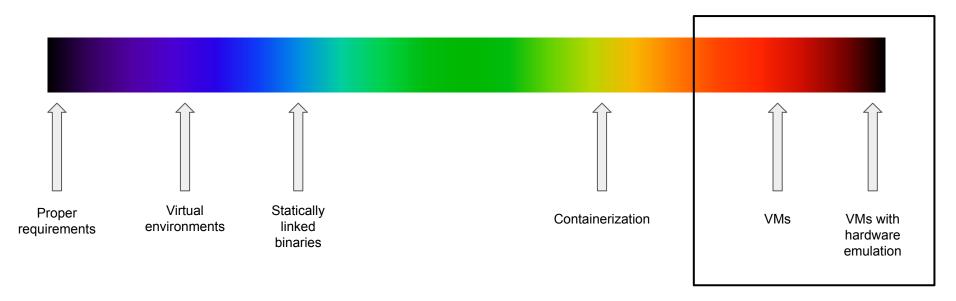
Virtual environments

- Work in a reproducible environment where libraries are the same for developers and for users. Each release has a virtual environment definition.
- Requires the user to set up and activate its own environment, and works only with some libraries (i.e. Python),
- Not a comprehensive solution and prone to human error \(\bigcup_{\infty}\) we stop here.

Statically linked binaries

- Works only for compiled or compilable languages \(\bigcup_{\infty}\) we stop here.

The "dependency hell" problem: solutions spectrum



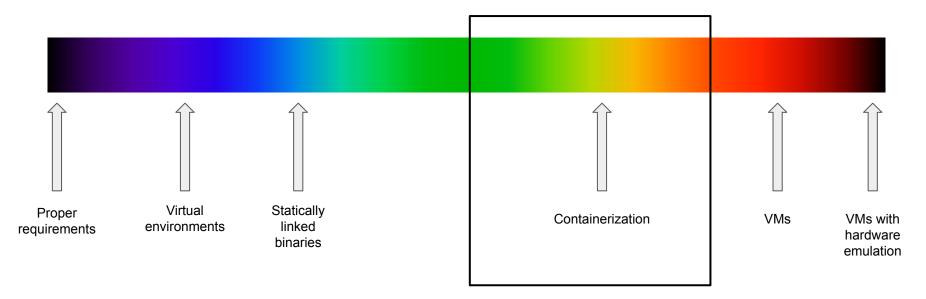
Virtual Machines with hardware emulation

Virtual Machines

- Works out-of-the box and does not touch the main OS;
- Allows to quickly test a given software / library;
- Need to download a (big) pre-built, *trusted* image (no "source" code);
- Requires pre-allocating dedicated memory at startup, and an entire boot;
- Not suitable for much more than just giving the software a try;
- You will not find much software packaged in this way.

... but we are on the right path. We want this kind of insulation!

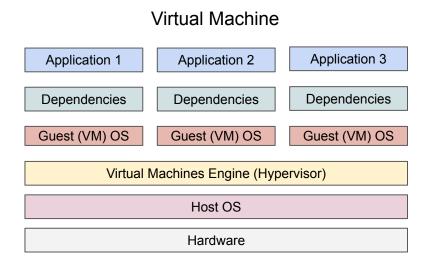
The "dependency hell" problem: solutions spectrum



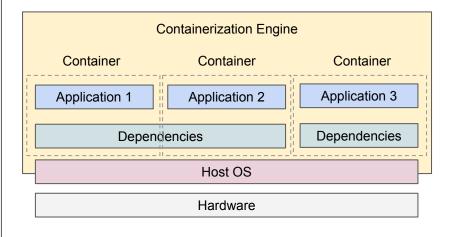
Containerization

You *might* think about it as a Virtual Machine in first approximation

→ but keep in mind that they are two completely different things



Containerization



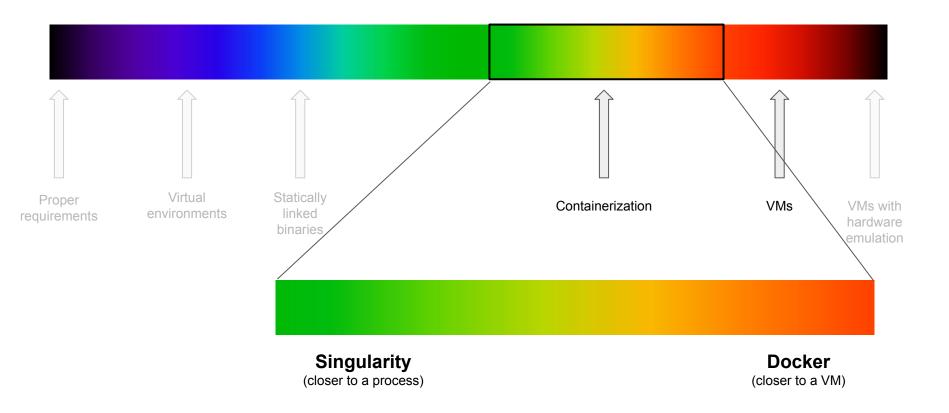
Containerization: the Virtual Machines alternative

The idea is to insulate a single process from your Operating System, and to:

- Let it live in its own space, including its own network;
- Let it have its own File System with its own libraries;
- Allow to natively access hardware without virtualization;
- Avoid booting an entire Virtual machine and to pre-allocate dedicated memory.

Different containerization solutions put more or less focus on these points

The "dependency hell" problem: solutions spectrum



Docker

- Modern containerization solution, open source
- Extremely popular, the "de facto" containerization standard
- Incremental File System
- Plenty of software on Docker Hub
- Native on Linux
- Almost native on Macs post-2011 and Windows 10 (through a light VM)

Docker Vs Singularity

Docker	Singularity
IT Industry standard	Scientific Computing
Running containers are seen as (micro)services	Running container are seen as processes
Containers have an IP address by default	Containers do not have an IP address by default
Extensive support for networking between containers	Limited or no support for networking between containers
Basically requires root access	Build as root, run as user
Limited HPC and parallelisation support	Full support for HPC use cases
Requires a daemon to orchestrate	Command line utility
Loads of orchestrators (docker-compose, kubernetes)	First alpha stage orchestrator (singularity-compose)

Docker Vs Singularity (more technical)

Docker	Singularity
<pre>docker run: Run a command in a new container</pre>	<pre>singularity run: Run the user-defined default command within a container</pre>
<pre>docker exec: Run a command in a running container</pre>	<pre>singularity exec: Run a command within a container</pre>
-	<pre>singularity instance: Manage containers running as services</pre>
Filesystem at runtime: completely insulated by default, use volumes to bind folders	Filesystem at runtime: only partially insulated by default, the directories \$HOME, /tmp, /proc, /sys, and /dev are mounted.
Environment at runtime: from scratch	Environment at runtime: the environment of the host
Network: the one of Docker engine, usenet-host to use the host network	Network: the one of the host

Tutorial start

We will now have a look about how to pull, run, build and share Docker containers

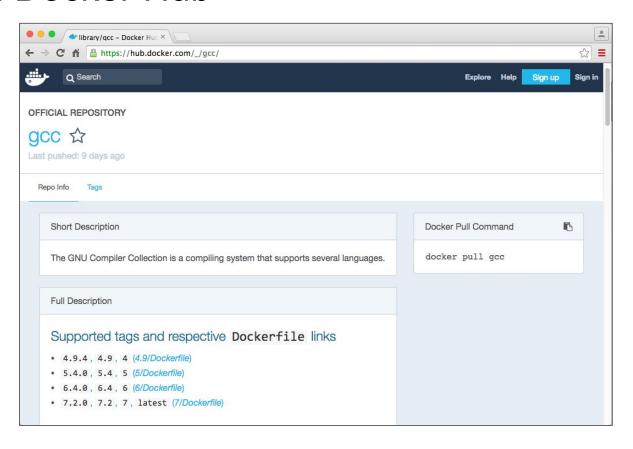
 You can use the Examples/step_by_step.sh script to follow more or less the same steps

```
$ ./step_by_step.sh

Will now pull gcc 5.4 Docker container

Command: docker pull gcc:5.4
Press enter to execute...
```

Gcc on Docker Hub



Gcc on Docker Hub (downloading)

- You are downloading a minimalistic Linux distribution (Debian Jessie, as we will see later) on which has been installed gcc (version 5.4).
- Thanks to Docker's incremental file system, another container based on Debian Jessie will not require to download/store it again.

Gcc on Docker Hub (downloaded)

```
$ docker pull gcc:5.4
5.4: Pulling from library/gcc
aa18ad1a0d33: Pull complete
15a33158a136: Pull complete
f67323742a64: Pull complete
c4b45e832c38: Pull complete
e5d4afe2cf59: Pull complete
4c0020714917: Pull complete
b33e8e4a2db2: Pull complete
c8dae0da33c9: Pull complete
Digest: sha256:e6ef7f0295b9d915f8521de360e30803bf8561cfb9cea8e320aa66761be8ec42
Status: Downloaded newer image for gcc:5.4
```

Terminology warning:

- image: a "file" from which you can run a container
- container: an "entity" run from an image

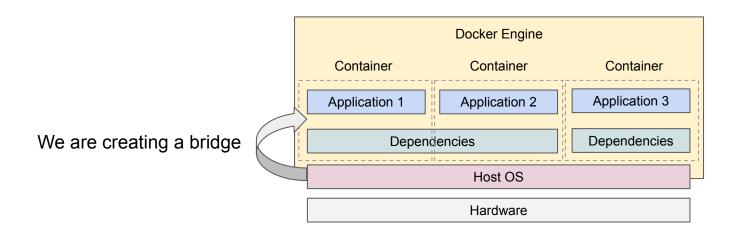
Run Gcc (5.4) with Docker

```
$ docker run gcc:5.4 gcc -v
Using built-in specs.
COLLECT_GCC=gcc
COLLECT_LTO_WRAPPER=/usr/local/libexec/gcc/x86_64-linux-gnu/5.4.0/lto-wrapper
Target: x86_64-linux-gnu
Configured with: /usr/src/gcc/configure --build=x86_64-linux-gnu --disable-multilib
--enable-languages=c,c++,fortran,go
Thread model: posix
gcc version 5.4.0 (GCC)
$
```

Share files with a Docker container: the volumes

The container is by definition insulated from your main (host) Operating System

- But you can make some folders visible from the containers as volumes (think about an usb pendrive)
- Just append "-v your_os_folder:path_inside_the_container" to docker command



Compile your code with Gcc (5.4)

Our test.c code:

```
#include<stdio.h>
int main()
{
    printf("I run a very complex simulation and the result is 42\n");
}
```

Compile your code with Gcc (5.4)

```
$ docker run -v$PWD:/data gcc:5.4 gcc -o /data/Test/test.bin --verbose /data/Test/test.c
Using built-in specs.
COLLECT GCC=gcc
COLLECT LTO WRAPPER=/usr/local/libexec/gcc/x86 64-linux-gnu/5.4.0/lto-wrapper
Target: x86 64-linux-gnu
Configured with: /usr/src/gcc/configure --build=x86_64-linux-gnu --disable-multilib
--enable-languages=c,c++,fortran,go
Thread model: posix
gcc version 5.4.0 (GCC)
COLLECT GCC OPTIONS='-o' '/data/Test/test.bin' '-v' '-mtune=generic' '-march=x86-64
[\ldots]
```

Run your code compiled with Gcc (5.4)

On your computer \rightarrow no!

```
$ Test/test.bin
-bash: Test/test.bin: cannot execute binary file
```

Inside the container → yes!

```
$ docker run -v$PWD:/data gcc:5.4 /data/Test/test.bin
ste@Stes-MacAir:Examples (master) $
I just ran a very complex simulation and the result is 42
```

Entering in the Gcc (5.4) container

Execute a (bash) shell in the container

```
$ docker run -t -i gcc:5.4 bash root@b9c1414bab3d:/#

You are root!
```

List the root directories

```
root@b9c1414bab3d:/# ls
bin boot dev etc home lib lib64 media mnt opt proc root run sbin srv
sys tmp usr var
```

Entering in the Gcc (5.4) container

List running processes

```
      root@b9c1414bab3d:/# ps -ef

      UID
      PID
      PPID
      C STIME TTY
      TIME CMD

      root
      1
      0
      1
      13:54 pts/0
      00:00:00 bash

      root
      8
      1
      0
      13:54 pts/0
      00:00:00 ps -ef
```

Get the container IP address

```
root@b9c1414bab3d:/# ip addr show dev eth0
[...]
inet 172.17.0.2/16 brd 172.17.255.255 scope global eth0
[...]
```

Entering in the Gcc (5.4) container

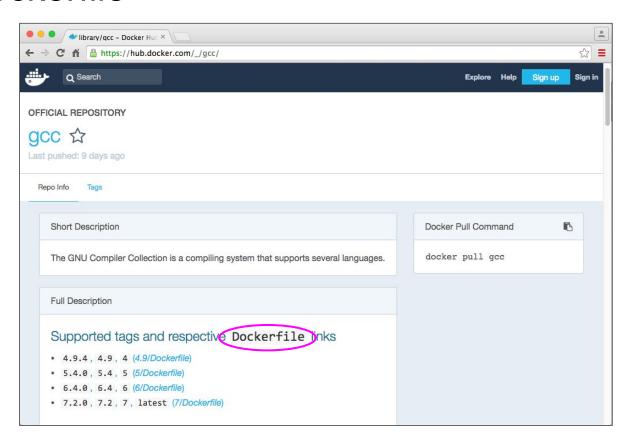
List running Docker containers (on another shell of your computer)

Exit the shell, and therefore the container

```
root@b9c1414bab3d:/# exit
$
```

When you exit a container, you lose every change to the container File System

The Dockerfile



The Dockerfile

- The Dockerfile is what defines a Docker Container. Think about it as its source code.
- When you build it, it generates a *Docker Image*. When you <u>run</u> a Docker Image, this "becomes" a *Docker Container*, as mentioned before.

```
FROM <base image>

RUN <a setup command>

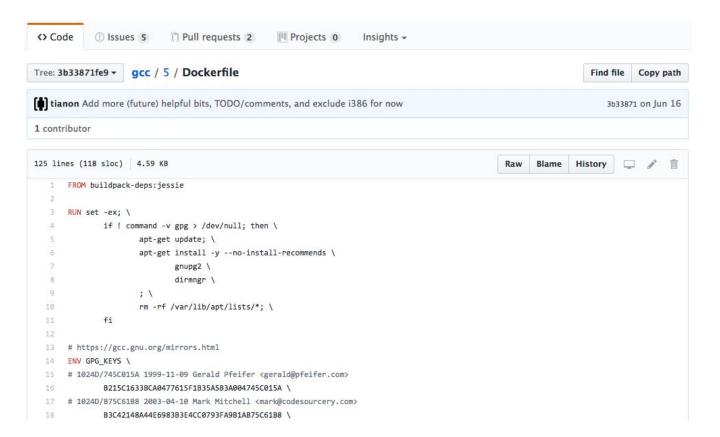
COPY <source file/folder on your OS> <dest file/folder in the container>

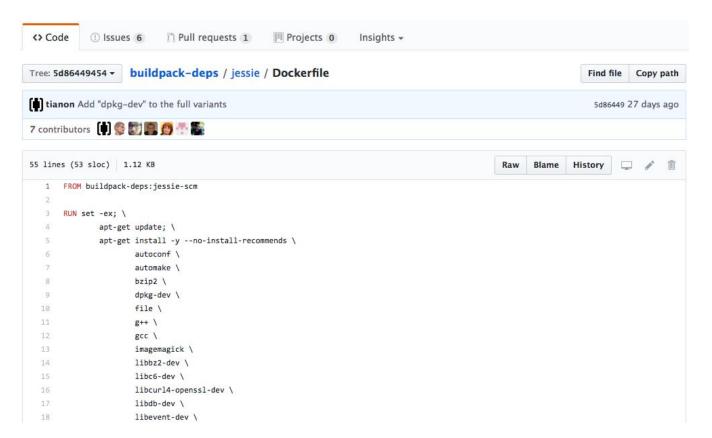
RUN <another setup command>
```

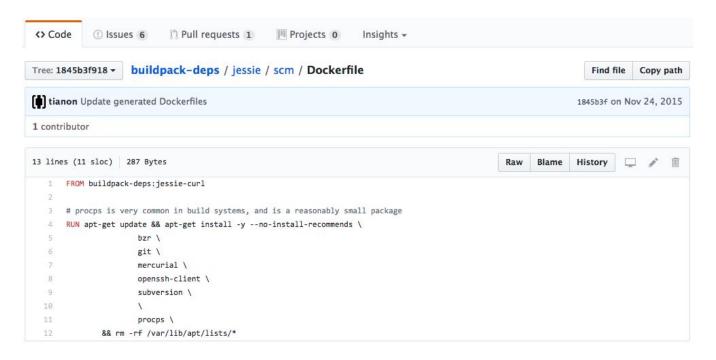
What is the Gcc (5.4) container built from?

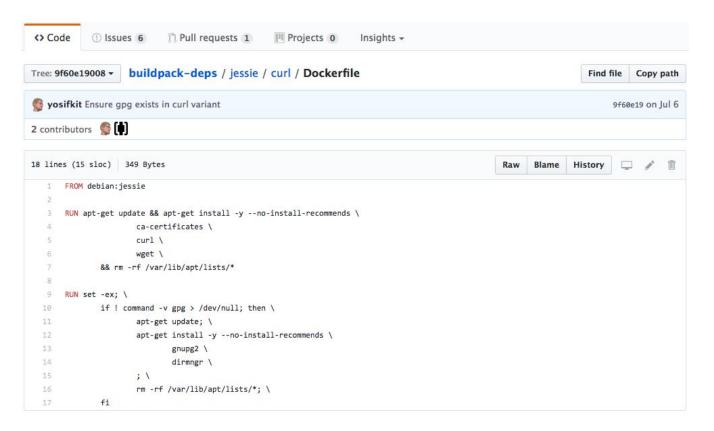
There is NO black magic in Docker.

Now that we know that its source code is in the Dockerfile, we can see on what the Gcc (5.4) image is *built from*.











We will now include and compile your test code directly from a Dockerfile

```
# Add the test code
COPY test.c /opt
# Compile the test code
RUN gcc -v -o /opt/test.bin /opt/test.c
```

Let's now build it with "test.c" and the Dockerfile files in a folder named "Test":

```
$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
Step 1/3: FROM gcc:5.4
 ---> b87db7824271
Step 2/3 : COPY test.c /opt
 ---> f5478f7830ee
Step 3/3 : RUN gcc -v -o /opt/test.bin /opt/test.c
 ---> Running in c839379f1fbe
Using built-in specs.
COLLECT GCC=gcc
[...]
Removing intermediate container c839379f1fbe
 ---> 2f0c6f89fdc0
Successfully built 2f0c6f89fdc0
Successfully tagged testcontainer:latest
```

..and we can run it:

```
$ docker run testcontainer /opt/test.bin
I just ran a very complex simulation and the result is 42
```

..and share it (old school):

```
$ docker save testcontainer > testcontainer.tar
```

```
$ docker load < testcontainer.tar</pre>
```

..and share it (Docker Hub):

```
$ docker tag testcontainer sarusso/testcontainer
$ docker push sarusso/testcontainer
The push refers to repository [docker.io/sarusso/testcontainer]
4e139ce93449: Pushed
8e5d12c6cc1e: Pushed
531d0aa62df3: Mounted from library/gcc
2ac9aba62fc1: Mounted from library/gcc
4e778218c153: Mounted from library/gcc
8f816dba9ff6: Mounted from library/gcc
7381522c58b0: Mounted from library/gcc
ecd70829ec3d: Mounted from library/gcc
d70ce8b0dad6: Mounted from library/gcc
18f9b4e2e1bc: Mounted from library/gcc
latest: digest: sha256:21563d1b6645af4cf73f01cc471b5f1a8bb902f7f1903bac4b9b878433eecf5e size: 2421
```

If we rebuild the testcontainer, the caching jumps in. It takes few seconds.

```
$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
Step 1/3: FROM gcc:5.4
 ---> b87db7824271
Step 2/3 : COPY test.c /opt
 ---> Using cache
 ---> f5478f7830ee
Step 3/3 : RUN gcc -v -o /opt/test.bin /opt/test.c
 ---> Using cache
 ---> 2f0c6f89fdc0
Successfully built 2f0c6f89fdc0
Successfully tagged testcontainer:latest
```

..this is possible thanks to *version hashes*

- An *hash* is the result of applying an hash function
- An hash function takes some input and generates a fixed-size output, like:

47e0b9046c241cc4653b876c2a8ab01341c00754

- A good hash function allows to virtually never have the same hash from different inputs.
- In both Git and Docker the input is your code, and and hash represents a unique (saved) state. Or, a particular point in your codebase "history".
- Then, it happens that hashes can be linked together, forming hierarchies.
- A tag is a friendly name for an hash.

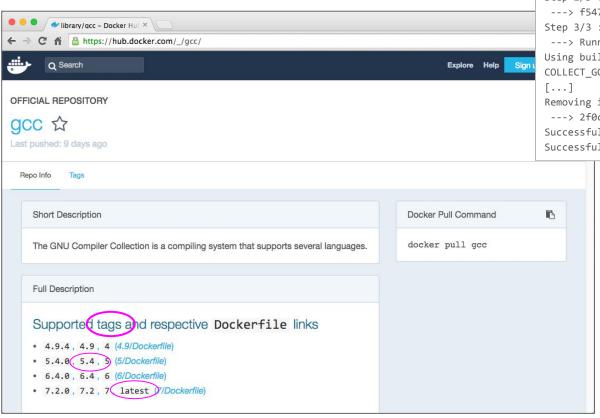
Let's have a look at the hashes for the first and second build

```
$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
Step 1/3: FROM gcc:5.4
 ---> b87db7824271
Step 2/3 : COPY test.c /opt
 ---> f5478f7830ee
Step 3/3 : RUN gcc -v -o /opt/test.bin /opt/test.c
 ---> Running in c839379f1fbe
Using built-in specs.
COLLECT GCC=gcc
[\ldots]
Removing intermediate container c839379f1fbe
 ---> 2f0c6f89fdc0
Successfully built 2f0c6f89fdc0
Successfully tagged testcontainer:latest
```

```
$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
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Step 2/3 : COPY test.c /opt
 ---> Using cache
---> f5478f7830ee
Step 3/3 : RUN gcc -v -o /opt/test.bin /opt/test.c
 ---> Using cache
 ---> 2f0c6f89fdc0
Successfully built 2f0c6f89fdc0
Successfully tagged testcontainer:latest
```

- Both Git and Docker implement versioning with hashes, which are fully deterministic, unlike version (incremental) numbers.
- In the Docker ecosystem everything is versioned
- For practical use, also the short hashes are allowed (and commonly used), which are the first 7 characters for Git (i.e. "47e0b90") and the first 12 for Docker.
- If by chance two hashes in the system starts with the same short hash, you will be required to enter one more character or the full hash.

One step back



\$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
Step 1/3 : FROM gcc:5.4
---> b87db7824271
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---> f5478f7830ee
Step 3/3 : RUN gcc -v -o /opt/test.bin /opt/test.c
---> Running in c839379f1fbe
Using built-in specs.
COLLECT_GCC=gcc
[...]
Removing intermediate container c839379f1fbe
---> 2f0c6f89fdc0
Successfully built 2f0c6f89fdc0
Successfully tagged testcontainer:latest

p.s. the tag "5.4" for the gcc Docker container is actually saying that the tag is "gcc:54". Sorry for this! :(

The hash for the tag "gcc:5.4" tag is "b87db7824271"

Where do you save your code and Dockerfile?

Where do you save your code and Dockerfiles?

..on a versioning system.

Where do you save your code and Dockerfiles?

..on a versioning system.

There is no other alternative.

Do not work without versioning.

Seriously, don't.

→ Use Dropbox or Google Drive if you think that more professional versioning tools, like Git, are an overkill.

The importance of versioning with Docker

Docker allows to have everything up and running, including dependencies etc. with a single command.

This command trigger a build with a given set of dependencies (the ones you wrote to install in the Dockerfile)

Over time, you will probably make changes in your Dockerfiles and in your code.

If you use a versioning system, you can jump back in time to a particular version/hash, build it, and it will run exactly as it was running at that time

For managing multiple container versions simultaneously you can use tags

The importance of versioning with Docker

Docker allows to have everything up and running, including dependencies etc. with a single command.

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For managing multiple container versions simultaneously you can use tags

Recap on Docker

- 1) With Docker, your code will build and run in the exact same way, on every operating system, virtually forever.
- 2) If you want to give the code that generates the magic "42" answer to someone, they will just need two commands* to have everything up and running:

```
docker build or pull docker run
```

Personal take

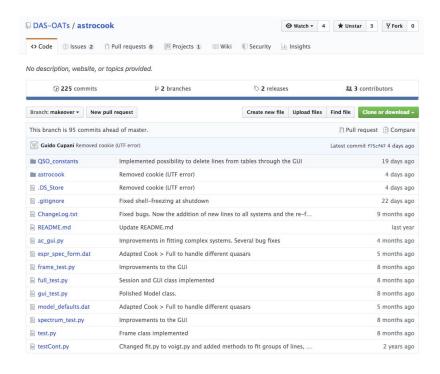
- A versioning systems protects you first of all from yourself
- Using Docker with a versioning system allows to reach full reproducibility, starting from a repository name and a short hash for a point in time/version.
- Using them even for small personal/research projects helps a lot
- If someone gives you a code without version control or that requires dependencies:
 - First, put it under version control;
 - Second, create a Dockerfile with all the commands and dependencies you will need to set it up (which you will need anyway, by the way).
- ..and no, tomorrow you will not remember how you did. No one does. :)

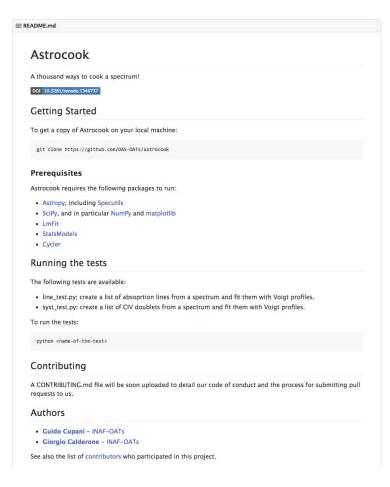
How about GUI programs?

Running a GUI program inside a container requires either a X11 server outside the container and forwarding the X11 socket, or other resorts like using VNC.

- Having a X11 server running outside a container and forward the X11 socket inside the container: ok on Linux, tricky on Mac, hard on Windows
- Better: embed a VNC server in the container and require just a VNC client
- Best: embed a WebVNC server in the container and require just a browser.

A thousand ways to cook a spectrum

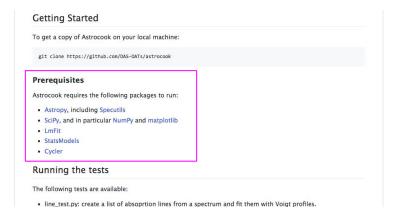




A thousand ways to cook a spectrum

Typical Scientific Code that requires non-trivial dependencies.

It has a GUI, meaning that it requires even other "implicit" dependencies



Ok, let's start to figure out how to install the dependencies.. on my 4 years old OS.

```
$ docker pull sarusso/astrocook
```

```
$ docker run -v$PWD:/data -p8590:8590 sarusso/astrocook
```

..and then open a browser on localhost:8590

Clone the Astrocook repo, then:

```
$ docker build -f containers/Docker/Dockerfile . -t astrocook
```

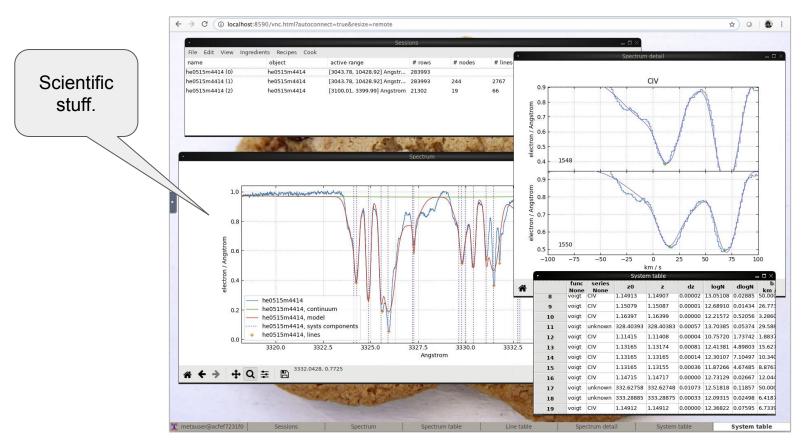
```
$ docker run -v$PWD:/data -p8590:8590 astrocook
```

..and then open a browser on localhost:8590

My browser

Practical example: Astrocook





Hope it helps:)

Questions?

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Talk repository: https://github.com/sarusso/ModernSoftwareDevelopment