Software containers

Or, the definitive solution for escaping the dependency hell and ensuring scientific reproducibility.

Stefano Alberto Russo - INAF / University of Trieste

Introduction

Software containers are lightweight, standalone, executable packages of software that include everything needed to run an application: code, runtime, system tools, system libraries and settings.

They bring basically the same benefits of virtual machines but require a fraction of their resources. For this reason, software containers are the perfect solution for providing reproducible test fast and flexible working environments.

Containers are a standard in the IT industry since many years, and are gaining traction in the scientific community as well.

This seminar will introduce the basics of software containerization using the Docker engine, how to avoid the common pitfalls when using them, and how to containerize scientific codes in order to make them both reproducible and easily shareable.

Why should you listen to me?

An hybrid profile:

- BSc in Computer Science
- MSc in Computational Physics

Started at CERN, as research fellow working on data analysis & Big Data

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 launched my own one :)

Now back into research:

- INAF and UniTS, working on resource-intensive data analysis
- adjunct prof. of computer science at University of Trieste
- plus, experienced consultant for a number of private companies

Pointers







The deal

- 1) I will use Docker as reference, but the concepts are 100% engine-agnostic.
- Always interrupt if you have question, doubs, something not clear, curiosities.
 Let's try to keep it interactive!
- 3) Over the talk, think about a concrete use case close to your work. We can discuss a few at the end.



Outline

- The dependency hell problem
 - Meet Mike
 - Solutions spectrum
- Containers for the win
 - Meet
 - Main concepts
 - Docker
- Containers hands-on
 - Using containers
 - Building your first container
 - Sharing containers

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→ Meet Mike

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.

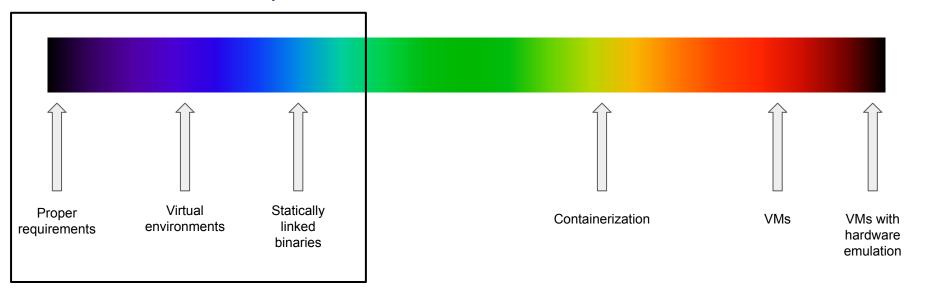
During this process, something goes wrong.

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.

→ Solutions spectrum



→ Solutions spectrum



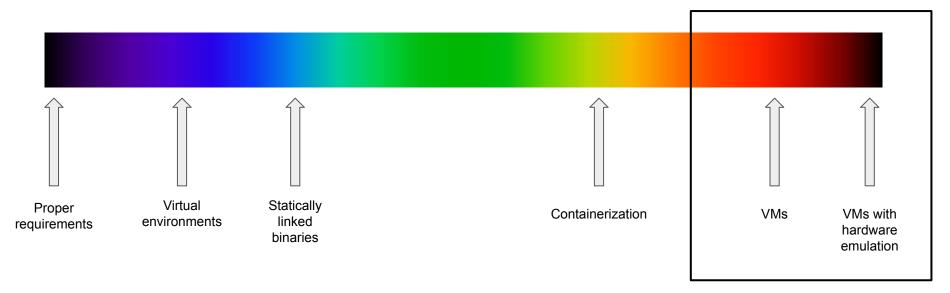
- → Proper requirements
- Carefully keep track of what libraries/OS features are used in development and report them on the documentation, for each release.
- Prone to human error we stop here.

- → 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 _____ we stop here.

- → Statically linked binaries
- Works only for compiled or compilable languages ——> we stop here.

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→ Solutions spectrum

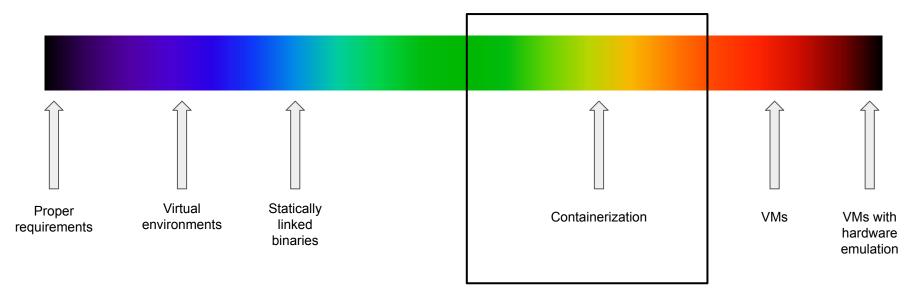


- → Virtual machines with hardware emulation
- Well... a bit of over-engineering. \(\bigcup_{\text{we}}\) we stop here.

- → 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.

cons > pros we stop here.

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

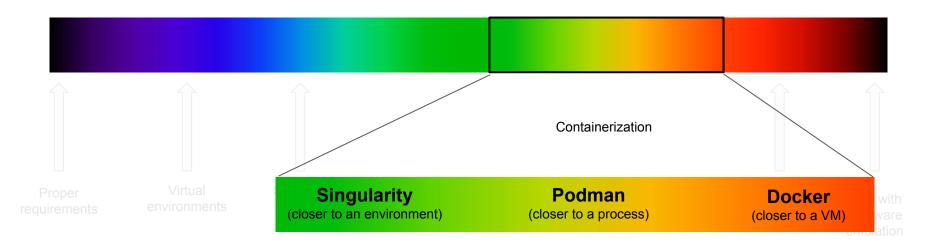


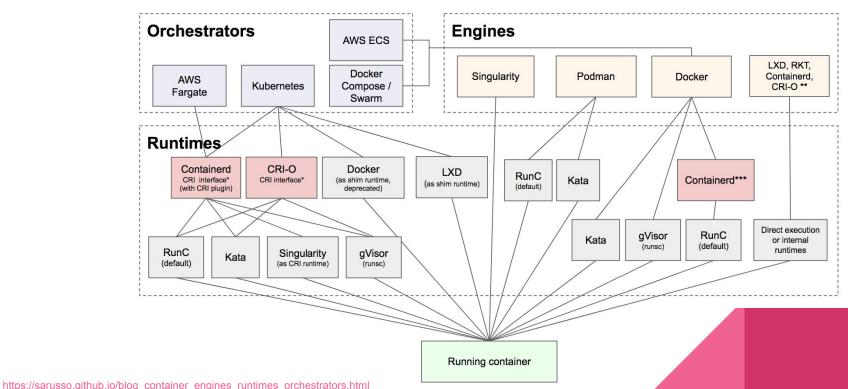
→ Containerization

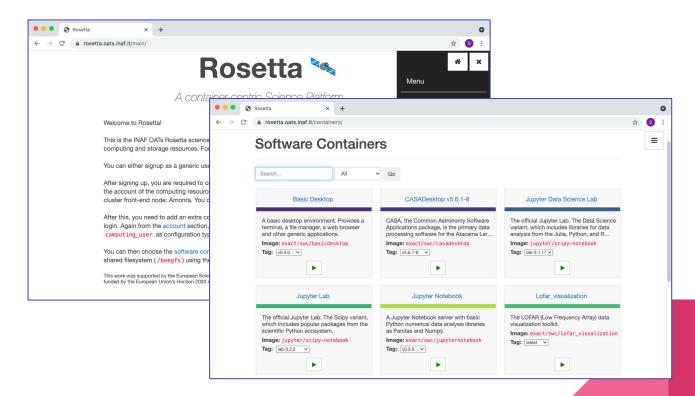
Containers are lightweight, standalone, executable packages of software that include everything needed to run an application:

- code
- runtime
- system tools
- system libraries
- settings etc.

Containers allow to reliably move and distribute software from one computing environment to another, without the burden of VMs.







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→ Meet Bill

Bill wants to install a new software.

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

Bill ask/Google for help and finds out that there is a container for it.

Bill pulls the container and runs it.

Bill immediately discovers that theat software is not suitable for his research, and finds a more appropriate one (as a container, of course!)

Bill spends the afternoon writing conclusions on his very important research using his new software while enjoying a hot cup of latte.



→ Meet Bill

Bill wants to install a new software.

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

Bill ask/Google for help and finds out that there is a container for it.

Bill pulls the container and runs it.

Bill immediately discovers that theat software is not suitable for his research, and finds a more appropriate one (as a container, of course!)

Bill spends the afternoon writing conclusions on his very important research using his new software while enjoying a hot cup of latte.

 \rightarrow be like Bill.



→ Main concepts

The idea of containers 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.

You might think about them as Virtual Machines in first approximation

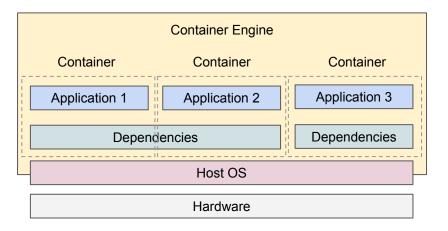
 \rightarrow but keep in mind that they are two completely different beasts.

→ Main concepts

Application 1 Application 2 Application 3 Dependencies Dependencies Guest (VM) OS Guest (VM) OS Virtual Machines Engine (Hypervisor) Host OS Hardware

Virtual Machines

Software Containers



→ Main concepts

How to run a container?

- 1) Get or build a container image (think about it as a file)
- 2) Run the image: this is your container

```
Usually: docker run my_container
```

..where "docker" can be replaced with your container engine of choice, e.g Podman.

Note: many engines, if cannot find the image locally, will automatically look online.

→ Main concepts

Example: Docker hello world!

\$ docker run hello-world

→ Main concepts

Example: Docker hello world!

```
$ docker run hello-world
ste@Stes-MacAir:INAF $ docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
2db29710123e: Pull complete
Digest: sha256:6d60b42fdd5a0aa8a718b5f2eab139868bb4fa9a03c9fe1a59ed4946317c4318
Status: Downloaded newer image for hello-world:latest
Hello from Docker!
This message shows that your installation appears to be working correctly.
```

→ Main concepts

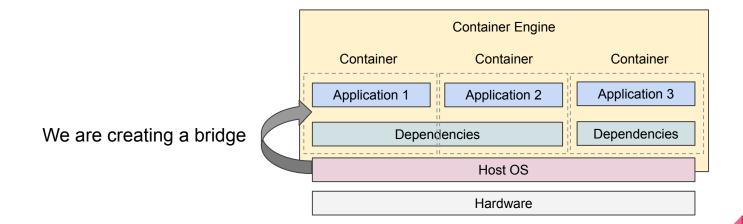
```
$ docker run -it python:3.8
```

→ Main concepts

```
$ docker run --entrypoint /bin/bash -it python:3.8
```

→ Main concepts

How to share files with a container? → **volumes**



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→ Main concepts

Example: make your home folder visible from within a container

```
$ docker run -it -v $HOME:/data python:3.8
```

→ Main concepts

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```
$ docker run -it -v $HOME:/data python:3.8

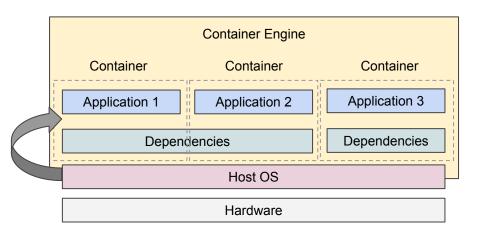
Python 3.8.12 (default, Dec 21 2021, 10:45:09)
[GCC 10.2.1 20210110] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import os
>>> os.listdir('/data')
['Applications', 'Desktop','Documents', 'Downloads', 'Dropbox', 'iCloud',
'Library', 'Movies', 'Music', 'Pictures', 'Public']
```

→ Main concepts

How to access servers* in a containers? → *port mapping*

*e.g. a Jupyter Notebook server

We are creating a bridge



→ Main concepts

Example: two Jupyter notebooks running with two Tensorflow versions

```
$ docker run -p 9001:8888 jupyter/tensorflow-notebook:tensorflow-2.4.1
```

```
$ docker run -p 9002:8888 jupyter/tensorflow-notebook:tensorflow-2.4.3
```

→ Main concepts

Performance aspects

Testing a package without a container, on OSX

```
$ python3 -m unittest discover

Ran 90 tests in 41.405s

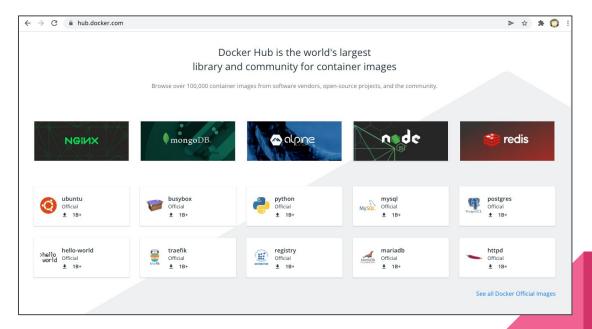
Testing a package inside a container on OSX: it is even faster!

$ python3 -m unittest discover

Ran 90 tests in 34.108s
```

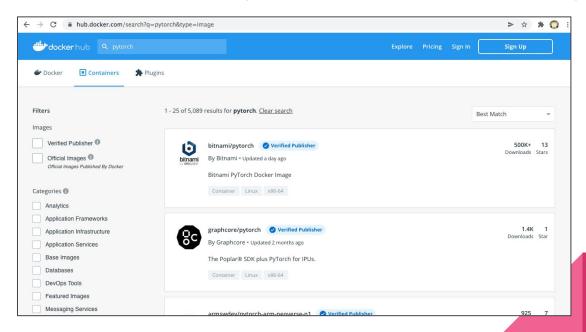
→ Main concepts

How to share containers? \rightarrow *registries* (the GitHub for software containers)



→ Main concepts

How to share containers? \rightarrow *registries* (the GitHub for software containers)



- → Docker
- Modern containerization solution, open source + freemium
- 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)
 - → Issues with new Apple M1 (ARM) chips!

- → Docker
- Relies on a system daemon to manage containers
- Running containers are seen as (micro)services
- Containers have an IP address by default
- Extensive support for networking between containers
- Requires a *privileged* user (do not expect to do a "docker run" on clusters)
- Loads of orchestrators (docker-compose, kubernetes..)

→ Docker

Common commands docker build: Build a container docker pull: Pull a container (from a registry) docker run: Run a container (and execute the default command, or a custom one) docker ps: List running containers docker exec: Run a command in a running container docker stop: Stop a running container docker rm: Remove a container

→ Docker

Isolation (to keep in mind)

Filesystem at runtime: completely isolated by default, use volumes to bind folders

Network: isolated within the Docker engine, use --net-host to use the host network

Environment at runtime: from scratch

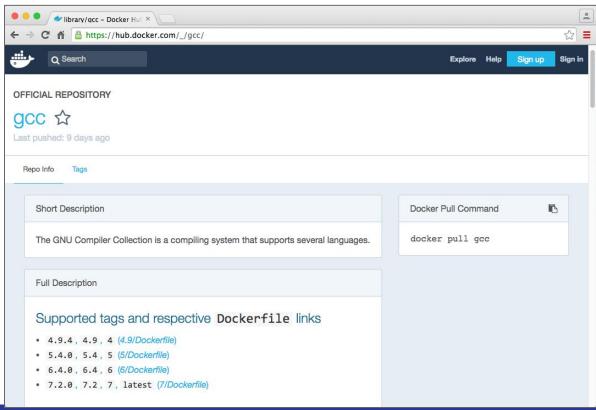
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- → Start
- If you want to follow, ensure you can run the hello world

\$ docker run hello-world

→ 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 reminder:

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

→ Run Gcc (5.4)

```
$ 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)
$
```

→ 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.bin --verbose /data/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
[...]
```

→ 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.bin
ste@Stes-MacAir:Examples (master) $
I just ran a very complex simulation and the result is 42
```

→ Enter in the Gcc (5.4) container

Execute a (bash) shell in the container

```
$ docker run -it 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
```

→ Enter 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
[...]
```

→ Enter in the Gcc (5.4) container

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

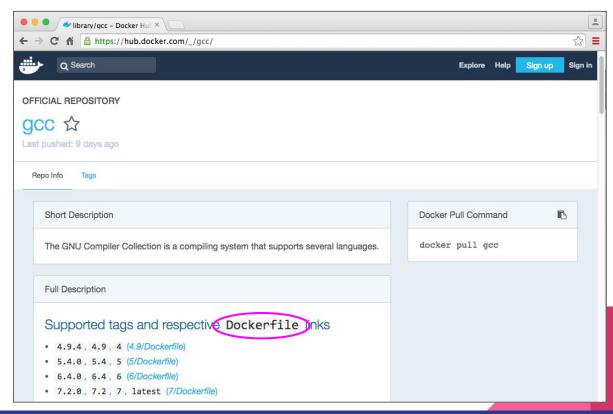
```
$ docker psCONTAINER IDIMAGECOMMANDCREATEDSTATUSPORTSNAMESb9c1414bab3dgcc:5.4"bash"3 seconds agoUp 1 secondfriendly_goodall
```

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



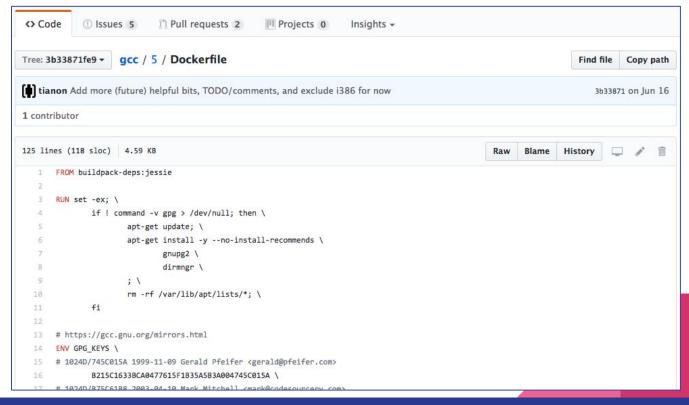
- → The Dockerfile
- The *Dockerfile* is what defines a Docker Container. Think about it as its source code.
- When you build it, it generates a Docker Image. When you run a Docker Image, this
 "becomes" a Docker Container, as mentioned before.

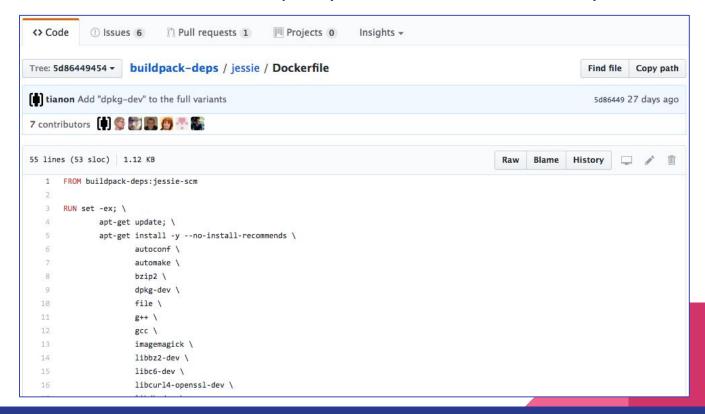
```
FROM <base image>
RUN <a setup command>
COPY <source file/folder on your OS> <dest file/folder in the container>
RUN <another setup command>
```

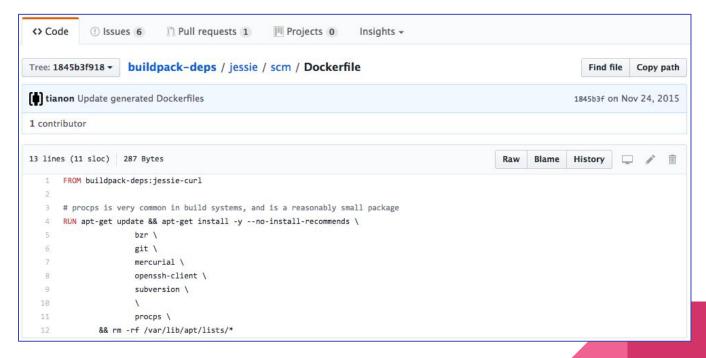
→ On what is the Gcc (5.4) container built upon?

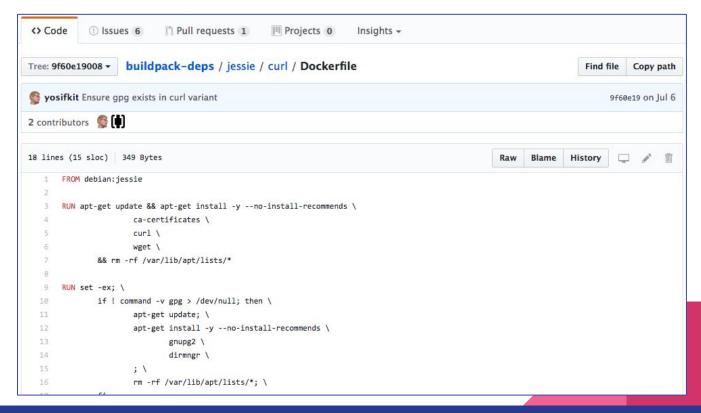
There is NO black magic in Docker.

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*.











→ Your first Dockerfile

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
```

→ Your first container

Let's now build it. Place the Dockerfile and the "test.c" in a folder named "Test", then:

```
$ 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
```

→ Your first container

..and run it:

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

→ Your first container

..and share it (old school):

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

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

→ Your first container

..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
```

→ Versioning: hashes, tags, etc.

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
 ---> h87dh7824271
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

- → Versioning: hashes, tags, etc.
- 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 get 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.

→ Versioning: hashes, tags, etc.

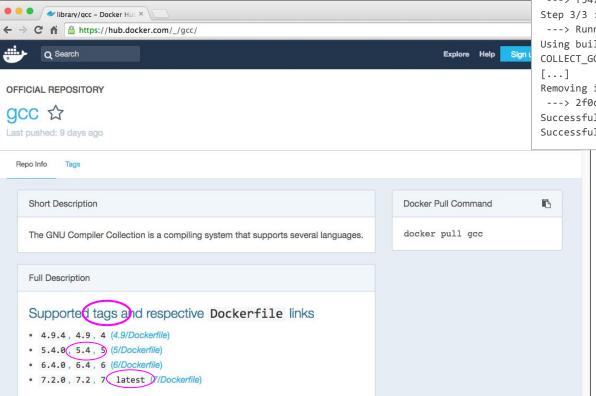
Let's have a look at the hashes for the first and second build

```
$ docker build Test -t testcontainer
Sending build context to Docker daemon 10.24kB
Step 1/3: FROM gcc:5.4
 ---> b87db7824271
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 ---> f5478f7830ee
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 ---> 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
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
```

- → Versioning: hashes, tags, etc.
- 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.

→ Versioning: hashes, tags, etc.



\$ docker build Test -t testcontainer
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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 Dockerfiles?

→ Where do you save your Dockerfiles?

..on a versioning system.

→ Where do you save your 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.

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

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For managing multiple container versions simultaneously, you can use **tags**

→ Recap

- 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

*plus some arguments

- → Recap
- 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 what you did.

No one does.:)

Thanks!

→ Questions?

