What place for the containers in the HPC world ?

06/28/17

Rémy Dernat – CNRS - ISE-M (CNRS/UM/IRD) / MBB platform LabEx CeMEB

JDEV2017

Containers

- Use some (~*recent*) "isolate" Linux capabilities:
  - chroot,
  - cgroups *(kernel > 2.6.24, 2008)*,
  - namespaces,
  - overlayFS *(kernel 3.18, Dec. 2014)*.

- + Possible Namespaces:
  - mnt (mount points, filesystems) *(kernel >= 2.4.19, 2002)*
  - pid (processes) *(Kernel >= 2.6.24, Jan. 2008)*
  - net (network stack) *(Kernel >= 2.6.24, Jan. 2008)*
  - ipc (InterProcess Communication) *(Kernel >= 2.6.19, Oct. 2006)*
  - uts (hostname / domainname) *(Kernel >= 2.6.19, Oct. 2006)*
  - user (UIDs/GIDs) *(complete in kernel >= 3.8, Feb. 2013)*
  - Cgroup Namespace (*Kernel >= 4.6 May 2016*)

Docker vs the rest of the world

- Some containers techs:
  - BSD Jails
  - Solaris Zones
  - OpenVZ
  - LXC/LXD
  - Docker
  - rkt
  - Systemd-nspawn
- In the HPC world, there are some initiatives but there are still rare.

Containers in production environments

- 1. Mainly used in **cloud environments** (Amazon, Google cloud...)
- 2. Moderate/weakly used in **standards datacenters**:
  - Proxmox and OpenVZ / LXC containers
  - Continuous development/integration/delivery/testing/deployment ↗
  - Except for some modern datacenters, but generally, these people are also using the cloud (point 1).
- 3. Poor usage in the **HPC** world (until… And except for... - *will see it later*...)

Why using containers in the HPC world ?

- **Mobility**: bring your working environment to the unfriendly HPC environment to benefit its hardware performances.
- Develop locally, build container, deploy at scale.

  Continuous Integration/Delivery/Deployment.

  DevOps aim: conciliates Ops and Devs.
- Less headaches for the HPC sysadmin (It is easy !), except for some containers techs/users that need additional security controls.

  → transfer partially the software stack responsibility to the user.

It leverages the user independence and its linux skills. To achieve this, the administrator should only give some good practices and recipes to help the user.

Why using containers in the HPC world ?

- **Reproducible Research ?**
  Recipe + Versioning + packaging + publishing/sharing

> ***Reproducibility*** *is the ability of an entire analysis of an experiment or study to be* ***duplicated****, either by the same researcher or by someone else working independently, whereas* ***reproducing*** *an experiment is called* ***replicating*** *it. Reproducibility and replicability together are among the main principles of the scientific method. (source: Wikipedia)*

Docker and its environment vs HPC environment

- 2 possible approaches :
  - Containers **orchestration with a job scheduler** inside each container (runner or master).
  - Classical **Job scheduler which distribute containers**.
- Docker orchestrators: Swarm, YARN, Mesos DC/OS, Kubernetes, etc...

  vs HPC Job Scheduler (SGE, Torque, SLURM, etc…)

  Oriented Docker *o*rchestrators hardly integrate within existing HPC environments with another job scheduler.

Docker and its environment vs HPC environment

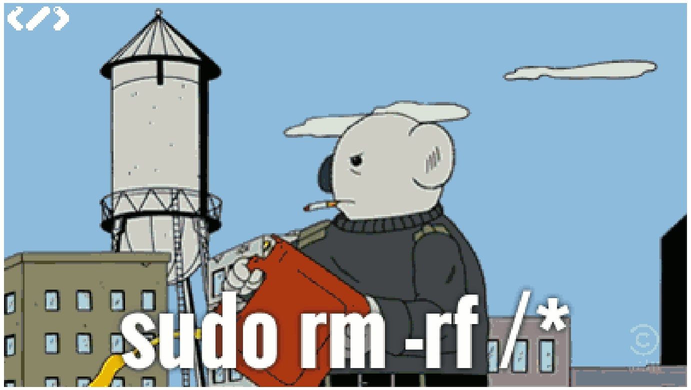
- Not HPC oriented. Created for the clouds:
  - **Micro-services, not “jobs”**...
  - The orchestrators distribute widely the containers without a true inquiry about the resources or scheduling and fair sharing.
  - Docker has **no HPC specific features**. It does not benefit the best of hardware/system performances (filesystem, network, specific accelerators (GPU, Xeon Phi...)).

Docker and its environment vs HPC environment - Security

- Not intended for multi-user use on the host(s)
  - Obvious security issues; the **docker daemon is running under *root***.

    Example :

```
$ docker run -ti -v /:/tmp/_root_host test_remy bash
# rm -rf /tmp/_root_host/
```



Docker and its environment vs HPC environment - Security

- Almost no certified images and secure images.
  - *“**30%** of the images on the Docker Registry contain vulnerabilities”*

    BanyanBlog – 2015

- *How to **secure** it ?*
  - Docker-ee (1), udocker (2), Moby project + LinuxKit,...
    - Image Analysis : Clair (CoreOS) (6), Docker Security Scanning, quay.io security analyses, ... ?
  - HPC focus: Shifter (3), Singularity (4), CharlieCloud (5)…

1. https://www.docker.com/enterprise-edition
2. https://github.com/indigo-dc/udocker
3. https://www.nersc.gov/research-and-development/user-defined-images/
4. http://singularity.lbl.gov/
5. https://github.com/hpc/charliecloud
6. https://coreos.com/clair

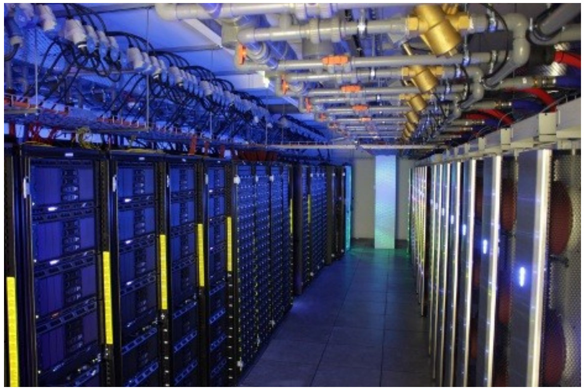
Comparison features table of Docker-like secure techs

Features	Docker-ee ($)	udocker	Shifter	Singularity	Charliecloud
Need a daemon	Yes	No	No	No	No
Permissions management	Yes	Not needed	Not needed	Not needed	Not needed
cgroups	Yes	No	Yes	No	No
Analyze images content	Yes (advanced edition ($$))	No	Yes / Partial	No	No
Access to the host devices	Yes (*--device* option)	No	No	Yes	Yes
True mapping of UIDs	No	Not for root	Not for root	Yes	No
All can be done from user	No (The admin needs to set permissions)	Yes	Yes (but it needs a gateway)	Yes (except bootstrap which requires root rights (*))	No
HPC ready	No	Yes (with some limitations)	Yes (and only for it (**))	Yes	Yes

(*) Can be done on a local machine and then transferred to the executing machine.
(**) it needs the corresponding infrastructure.

The containers in the HPC landscape

- Custom scripts
- Some initiatives :
  - Tight Integration with docker in HTCondor (*Docker Universe Applications*)
  - Slurm cgroups
  - The Dockstore
  - cHPC
  - Shifter
  - Charliecloud
  - Singularity



HTCondor : Docker Universe Applications

- Tight integration of Docker containers with **HTCondor**.
  - Pull the container from a registry,
  - mount a scratch directory within the container which contains every input/ouput files,
  - Execute a line defined in the submit script or the command defined by the Dockerfile.
  - Container is removed at the end of the job (regardless the final state of the job).

```
universe                = docker
  docker_image            = debian
  executable              = /bin/cat
  arguments               = /etc/hosts
  should_transfer_files   = YES
  when_to_transfer_output = ON_EXIT
  output                  = out.$(Process)
  error                   = err.$(Process)
  log                     = log.$(Process)
  request_memory          = 100M
  queue 1
```

The Dockstore

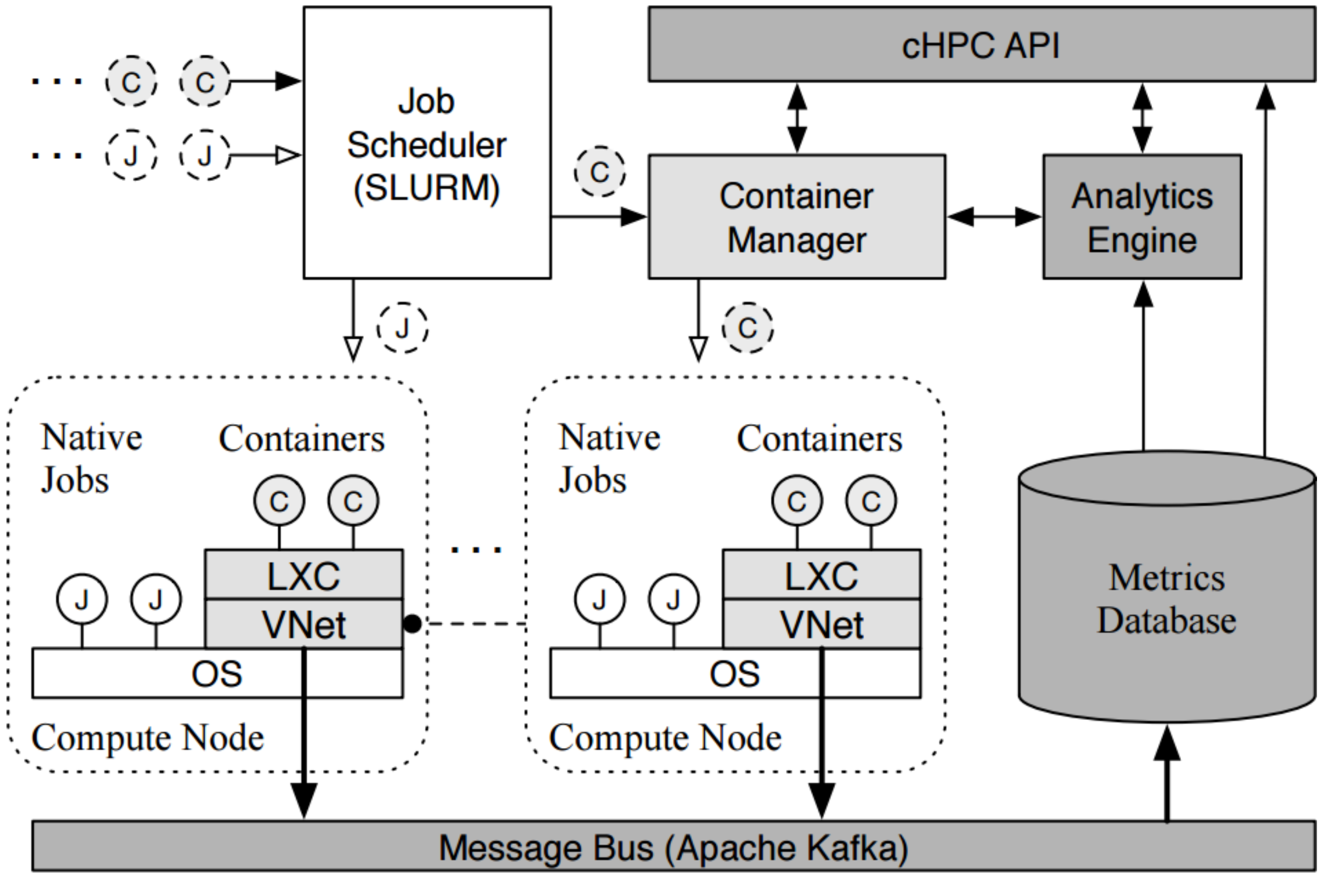
- Based on Docker, and a RESTful API with a java tool https://dockstore.org/
- Allows us to use almost pretty certified images focused on a science aim (for bioinfo purpose, see also BioShaDock / bioboxes ...).
- ICGC PanCancer Analysis of Whole Genomes cancer genomics project

  « At its peak, 14 cloud and HPC environments were utilized with over 16,000 cores in total, resulting in a cumulative dataset of nearly 1 Petabyte in size. »

The Dockstore

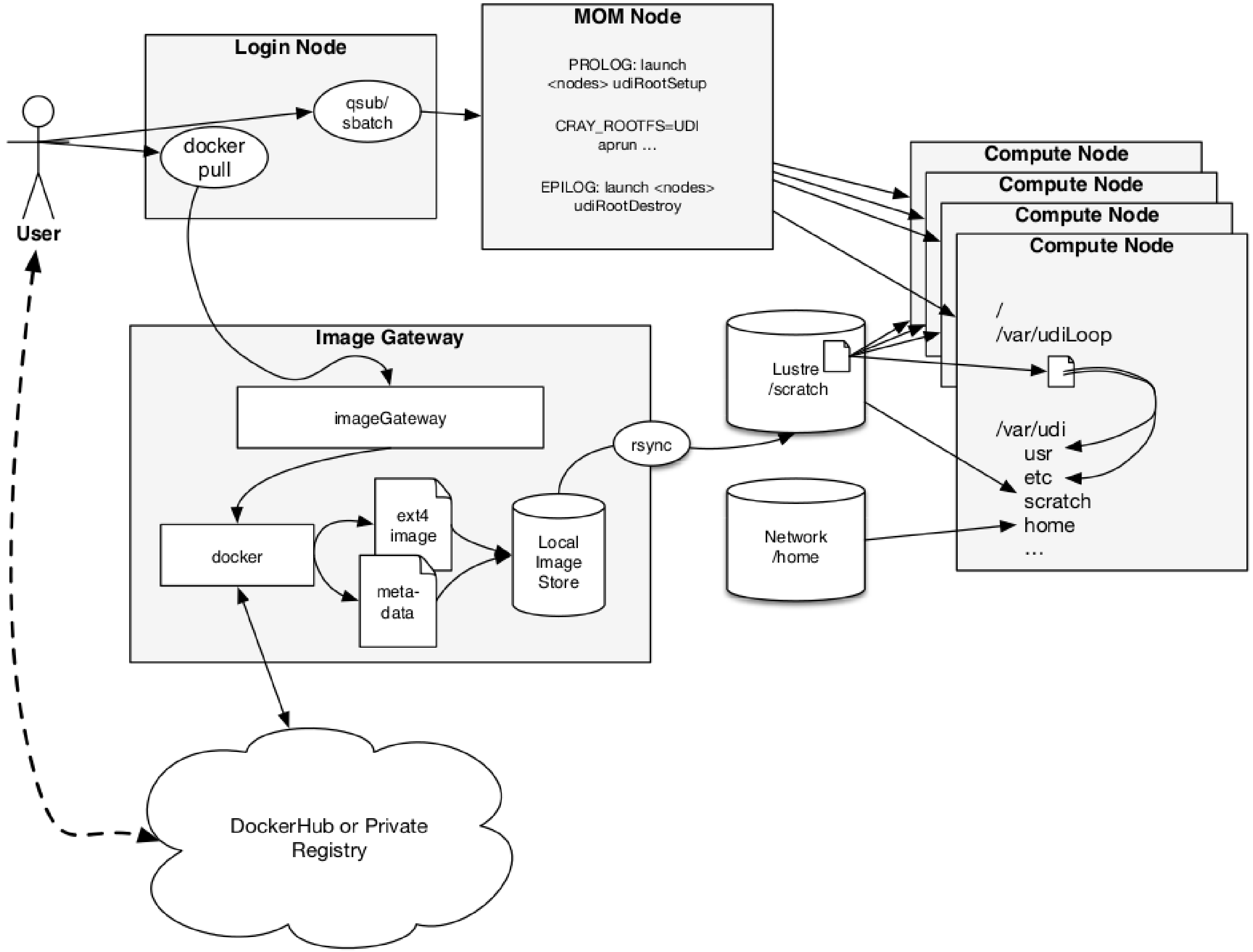
- Defines some standards formated in WDL/CWL (YAML)
  - Describes the container, who is the maintainer, what it does, its IOs (it is possible to describe an entire workflow), how to use it, and **what resources are needed for its execution**.
- Needs the Docker daemon on all executing nodes.

cHPC



Weidner, O., Atkinson, M., Barker, A., & Filgueira Vicente, R. (2016, June). Rethinking High Performance Computing Platforms: Challenges, Opportunities and Recommendations. In Proceedings of the ACM International Workshop on Data-Intensive Distributed Computing (pp. 19-26). ACM.

Shifter



Jacobsen, D. M., & Canon, R. S. (2015). Contain this, unleashing docker for hpc. Proceedings of the Cray User Group.

Shifter

- **Purpose**: anyway, everybody use Docker(…); How can we secure it to integrate these containers in our HPC cluster ?
- Developed at **NERSC** (National Energy Research Scientific Computing Center)
- A bit less complex than cHPC, but it is still a bit complex (…).

  Shitfer requires a **gateway** to convert the Docker image to a standard linux file (typically an ext4 image file after extracting Docker layers to a tarball). The gateway analyzes the content of the image to check any security issue.

Shifter

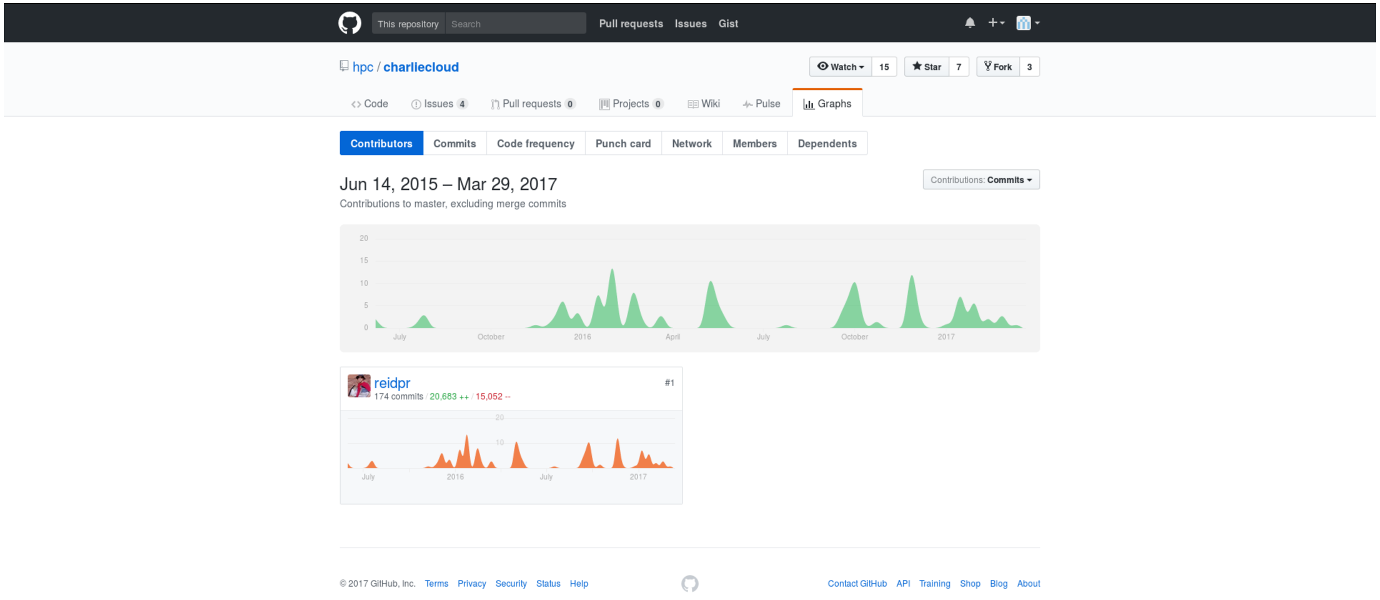
- Then, the **gateway** distributes the image over the **nodes**. The executing nodes mount it with a **loop device** and access to other paths (eg /output) with bind-mounts.
- The final image is mounted read-only for most of the paths and some operations are forbidden (setuid...).
- Works with SLURM, Torque.

Charliecloud

- https://hpc.github.io/charliecloud/
- Developed at Los Alamos National Laboratory
- Uses only 2 namespaces : *mount* and *user*
- Based on Docker for the container creation (*Dockerfile*),
- A little C+bash code (~500 lines) + bind mounts to execute the containers,
- User escalation is not possible,
- Charliecloud workflow:
  - *Dockerfile → the user*,
  - Building the image + tarball conversion → root,
  - Unpack tarball / Bind-mount / Execution → the user,

Charliecloud

- Use the host network,
- Not heavily maintained with only **one contributor** (Reid Priedhorsky),
- Limited in term of functionalities.



Singularity

(c) Gregory M. Kurtzer

Singularity

- http://singularity.lbl.gov/
- Mostly developed par Gregory M. Kurtzer (CentOS, Warewulf, …) at Lawrence Berkeley National Laboratory,
- Motto BYOE (Bring You Own Environment),
- The container is **only one file**,
- Developed with HPC in mind: MPI, CUDA (…) !
- Pulling from docker to build a singularity container is possible ! As well as Dockerfile conversion to a Singularity Spec file.
- Possibility to push the image in a singularity hub or even in a docker registry (docker hub, local…).
- Integrates smoothly with any Job Scheduler.

Singularity

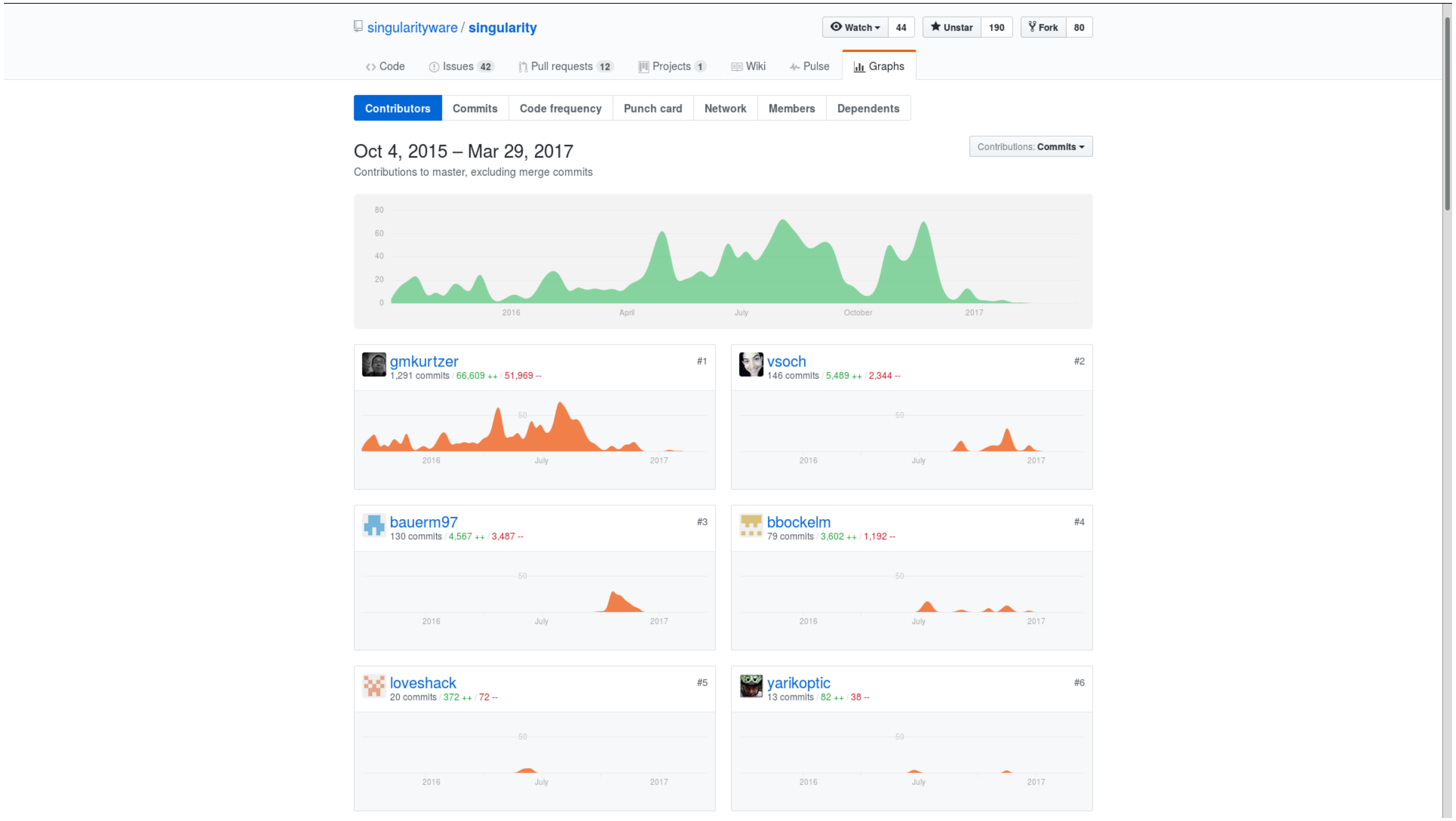
- True mapping of UID and GID inside/outside the container,
- User escalation is not possible,
- No (root) daemon,
- Possibility to include unit test.
- Singularity workflow:
  - *Dockerfile → the user*,
  - Creating/Building the image → root *(*)*,
  - Execution → the user,

(*) But you can build it on your local machine and then transfer it to a cluster as it is only one file !

- Possibility to use Pipe:

```
cat /path/to/python/script.py | singularity exec \
/tmp/Demo.img python
```

Singularity - activity



Singularity Spec File (.def)

sudo singularity create –size 2048 file.img

sudo singularity bootstrap file.img file.def

Header, %setup, %post, %test, %files, and %runscript sections

```
Bootstrap: docker
From: ubuntu:latest
IncludeCmd: yes

%runscript
    echo "I can put here whatever I want to happen when the user runs my container!"
    exec echo "Hello " "$@"
%post
   echo "Here we are installing software and other dependencies for the container!"
   apt-get update
   apt-get install -y git vim
```

Reproducibility

- **Reproducibility**
  - What we want in Science (reproducible research),
  - Undeniable advantages for the containers,
  - But… *Will see it later*
- **Versioning** and **sharing** simple files to be able to rebuild the same image:
  - *Dockerfile* for Docker
  - *Def/Specification file* for Singularity
  - Registries to push and share images.

Reproducibility

- What could **change** results between the host and the container (on the same host) ?
  - **Libraries** (used, versions…),
  - Compilation if needed (gcc ?, options, versions…),
  - **Environment variables**,
  - **External resources**:
    - Programs called (present or not, version...),
    - Downloads (the image, codes and packages…),
    - (non) Mounted filesystems (local bind, nfs…),
    - Random numbers,
    - Accesses and permissions with other programs and on resources :
      - Competitions, security (apparmor/selinux/seccomp profiles), …
- How to **solve** these problems (except for random numbers) ?
  - Using a .Spec file/Dockerfile, **running tests** (checksums, ldd (libraries), test section, scripts), **local resources**, and removing/controlling restrictions/checking accesses….

Reproducibility

- What could **change** results between the host and the container (on a different host) ?
  - *Each point from previous slide* +,
  - The **kernel version** and **loaded drivers** (presents ?, versions...),
  - The **processor** (brand (Intel/AMD), type/architecture (amd64 ? arm ? floating point precision...), available/activated features (AVX, SSE…)...), endianness ?,
  - Specific **local configurations**:
    - Local time, locales, encoding,
    - Network configuration (network stack, DNS…),
    - Sourced files
    - …
- How to **solve** all these problems ?
  - See previous slide → **tests**...

Performances and reproducibility

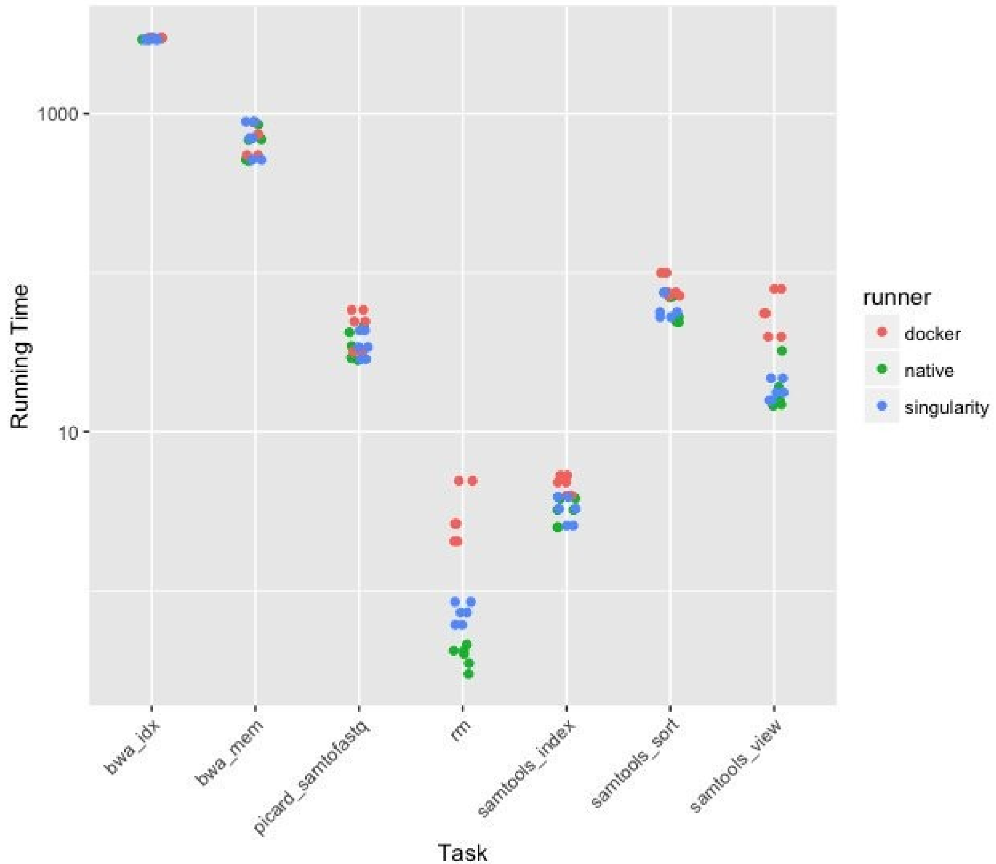
- Comparing reproducibility tests between **bare-metal** vs **singularity** vs **docker** vs **lxc**:
  - **Building a binary** and checking it with sha1sum and libraries with ldd:
    - Gives the **same results on a similar host** (sha1sum and libraries if it has been built with the same distro, the same version of gcc and in the same way).
    - A binary compiled on the host and then transferred on the container gives the same results (HPL linpack benchmarks) as if it was built on the container.

Performances and reproducibility

- Comparing some benchmarks between **bare-metal** vs **singularity** vs **docker** vs **lxc**:
  - Checking **startup** benchmarks,
  - Checking **network** benchmarks,
  - Checking **CPU** benchmarks,
  - Checking **HDD** IOs benchmarks,
  - Checking **Memory** IOs benchmarks,
  - Checking **GPU** benchmarks,

    https://github.com/remyd1/containers-benchs/

Jonathan Dursi – bioinfo tools benchmarks Singularity vs Docker and Native



(c) Jonathan Dursi. Y Axis in seconds