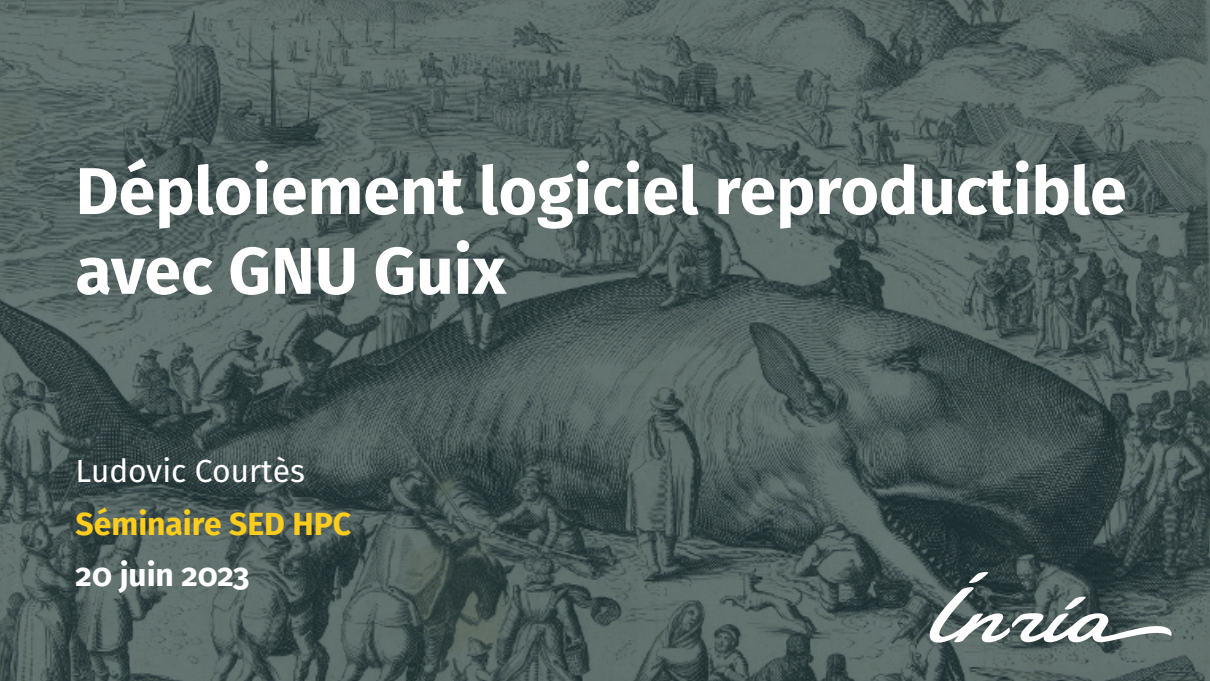




Déploiement logiciel reproductible avec GNU Guix

Ludovic Courtès

Séminaire SED HPC

20 juin 2023

Inria

- 
- ▶ Guix started in **2012**
 - ▶ tools for **reproducible software deployment**
 - ▶ runs standalone (Guix System) or atop a **GNU/Linux** distro
 - ▶ **≈23,000 packages**, all free software
 - ▶ **≈100 monthly contributors**

<https://hpc.guix.info>

- 
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 - ▶ **Guix-HPC effort (Inria, MDC, UBC, UTHCS) started in 2017**

<https://hpc.guix.info>

- ▶ **PlaFRIM** (FR): Inria Bordeaux (3,000+ cores)
- ▶ **GriCAD** (FR): Grenoble (1,000+ cores)
- ▶ **GLICID** (FR): Nantes (4,000+ cores)
- ▶ **Grid'5000** (FR): 8 sites (12,000+ cores)
- ▶ **Max Delbrück Center** (DE): 250-node cluster +
workstations
- ▶ **UMC Utrecht** (NL): 68-node cluster (1,000+ cores)
- ▶ ...

1. Robust deployment.

```
guix install gcc-toolchain openmpi hwloc
```

```
source ~/.guix-profile/etc/profile
```

```
guix package --roll-back
```

guix **shell** python python-numpy

```
guix shell python python-numpy \  
-- python3 -c 'import numpy'
```

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

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

```
guix shell --container \  
  --manifest=my-packages.scm
```

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

```
bob@laptop$ guix shell --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 shell --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 shell --manifest=my-packages.scm ...
```



travel in space *and* time!

Redeploy environments: 2 files, 2 commands

1. `guix describe -f channels > channels.scm`
2. `guix time-machine -C channels.scm -- \`
`shell -m manifest.scm`



CONDA



🚨 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

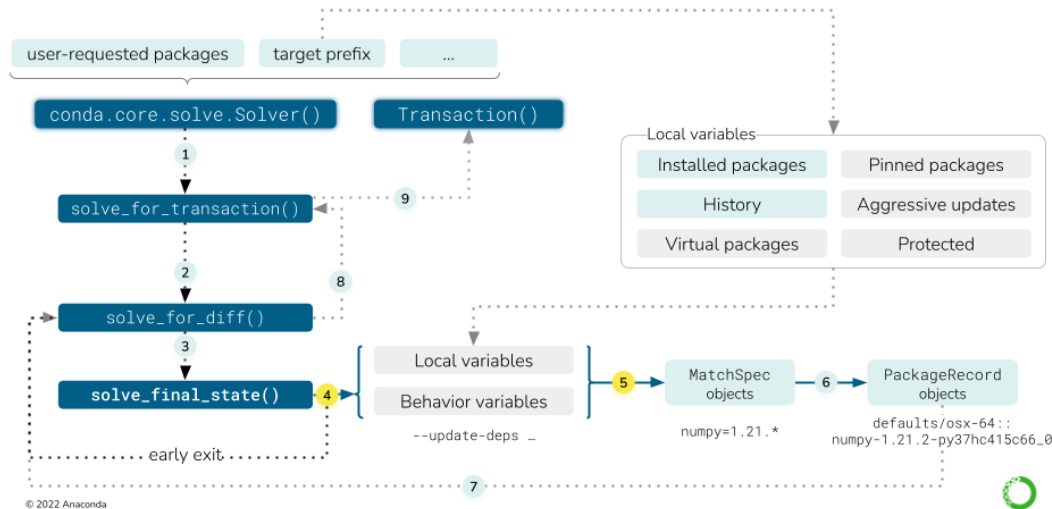
#11481 opened 6 days ago by chissg

🚨 Installation issue: boost **build-error**

💬 1

#11467 opened 7 days ago by abc19899

Inside the Solver: formulating the problem



```

$ wget -qO /tmp/pytorch.zip https://files.pythonhosted.org/pack
$ unzip -l /tmp/pytorch.zip | grep '\.so'
    29832  06-12-2021  00:37  torch/_dl.cpython-38-x86_64-linux
    29296  06-12-2021  00:37  torch/_C.cpython-38-x86_64-linux-
372539384  06-12-2021  00:37  torch/lib/libtorch_cpu.so
    43520  06-12-2021  00:37  torch/lib/libnvToolsExt-3965bdd0.
28964064  06-12-2021  00:37  torch/lib/libtorch_python.so
    46351784  06-12-2021  00:37  torch/lib/libcaffe2_detectron_ops
1159370040  06-12-2021  00:37  torch/lib/libtorch_cuda.so
    4862944  06-12-2021  00:37  torch/lib/libnvrtc-builtins.so
    168720  06-12-2021  00:37  torch/lib/libgomp-a34b3233.so.1
    116240  06-12-2021  00:37  torch/lib/libtorch.so
    523816  06-12-2021  00:37  torch/lib/libcudart-80664282.so.1
    222224  06-12-2021  00:37  torch/lib/libc10_cuda.so
    36360  06-12-2021  00:37  torch/lib/libshm.so
    47944  06-12-2021  00:37  torch/lib/libcaffe2_module_test_d
22045456  06-12-2021  00:37  torch/lib/libnvrtc-08c4863f.so.10
    12616  06-12-2021  00:37  torch/lib/libtorch_global_deps.so
https://hpc.guix.info/blog/2021/09/whats-in-a-package/

```

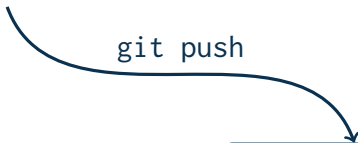
(define python
 (package ...))

test



guix build python
/gnu/store/...-python-3.9.6

git push



Git repository

(define python
 (package ...))

test

guix build python
/gnu/store/...-python-3.9.6

git push

Git repository

guix pull

user

```
graph TD; A["(define python (package ...))"] -- test --> B["guix build python /gnu/store/...-python-3.9.6"]; B -- "git push" --> C["Git repository"]; C -- "guix pull" --> D["user"];
```

(define python
 (package ...))

test

guix build python
/gnu/store/...-python-3.9.6

git push

guix pull

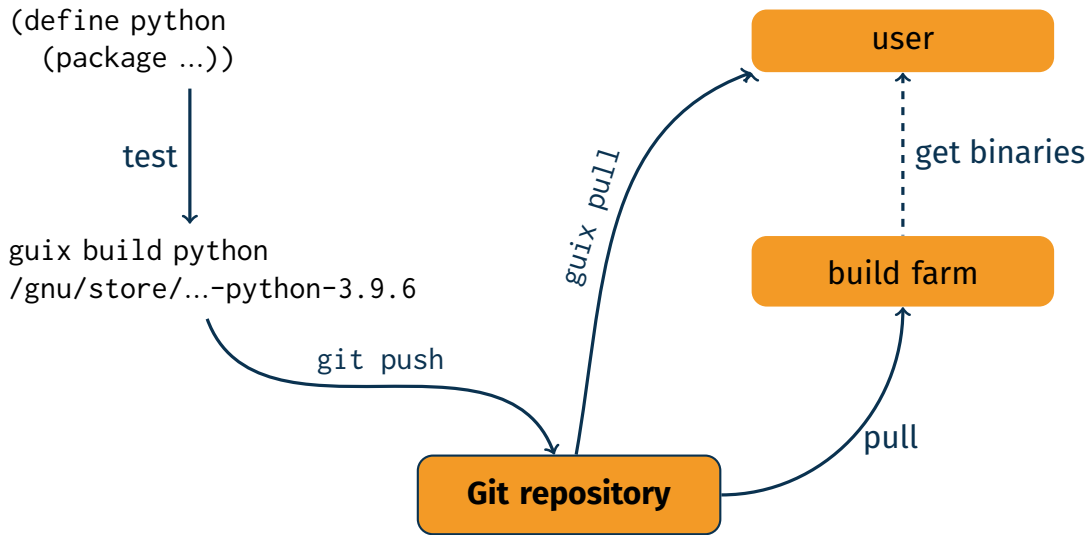
Git repository

user

get binaries

build farm

pull



build processes

chroot, separate UIDs

client commands

```
guix build hello
```

build daemon

build processes
chroot, separate UIDs

client commands

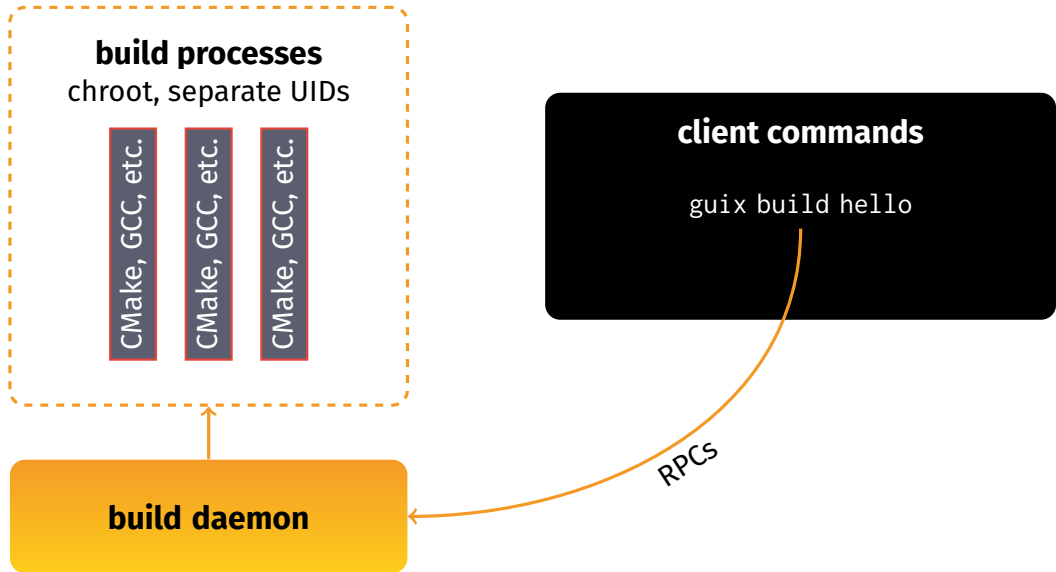
guix build hello

build daemon

RPCs

```
graph TD; A[client commands] -- RPCs --> B[build daemon];
```

The diagram illustrates the interaction between three components. At the top right, a black rounded rectangle labeled 'client commands' contains the text 'guix build hello'. At the bottom left, an orange rounded rectangle labeled 'build daemon' is shown. A curved orange arrow points from the 'client commands' box to the 'build daemon' box, with the label 'RPCs' written along the curve. In the top left, a dashed orange rounded rectangle labeled 'build processes' contains the text 'chroot, separate UIDs'. This box is not connected to the other components by arrows.



Channel	Commit
https://gitlab.inria.fr/guix-hpc/guix-hpc.git	9f5bbe50145056442ddc488babb9049dc6b3fae6
https://git.savannah.gnu.org/git/guix.git	03b463b68ba62b0b6f11a585240829fddef37f48

Builds of evaluation #6100591  

All 10  Scheduled 0  Succeeded 8  Failed 2

ID	Specification	Completion time	Job	Name	System	Log
  132227	guix-hpc	5 hours ago	gcvb-felsocim-0.0.1-git.6b03aec	gcvb-felsocim-0.0.1-git.6b03aec	x86_64-linux	raw
  132226	guix-hpc	5 hours ago	gcvb-1.0.0	gcvb-1.0.0	x86_64-linux	raw
  132225	guix-hpc	5 hours ago	python-dash-bootstrap-components-0.7.1	python-dash-bootstrap-components-0.7.1	x86_64-linux	raw
  132224	guix-hpc	5 hours ago	python-dash-defer-js-import-0.0.2	python-dash-defer-js-import-0.0.2	x86_64-linux	raw
  132219	guix-hpc	5 hours ago	python-pyamg-4.0.0	python-pyamg-4.0.0	x86_64-linux	raw
  132220	guix-hpc	5 hours ago	python-torch-diffeq-0.2.2	python-torch-diffeq-0.2.2	x86_64-linux	raw
  132218	guix-hpc	5 hours ago	python-torch-vision-0.2.2	python-torch-vision-0.2.2	x86_64-linux	raw
  132222	guix-hpc	5 hours ago	ddmpy-0.1	ddmpy-0.1	x86_64-linux	raw
  132221	guix-hpc	5 hours ago	python-ttpty-1.2	python-ttpty-1.2	x86_64-linux	raw
  132223	guix-hpc	5 hours ago	python-dash-4.0.0	python-dash-4.0.0	x86_64-linux	raw

<https://hpc.guix.info/blog/2023/03/contiguous-integration-and-continuous-delivery-for-hpc/>

2. Flexibility.

- ▶ <https://github.com/guix-science/guix-science>
 - ▶ RStudio Server, JupyterLab, Grid Engine, ...
- ▶ <https://gitlab.inria.fr/guix-hpc/guix-hpc>
 - ▶ HPC run-time support and linear algebra libraries (StarPU, Maphys, ...)
- ▶ <https://gitlab.inria.fr/guix-hpc/guix-past>
 - ▶ vintage packages (Python 2.x, NumPy, etc.)
- ▶ ...

<https://hpc.guix.info/browse>

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

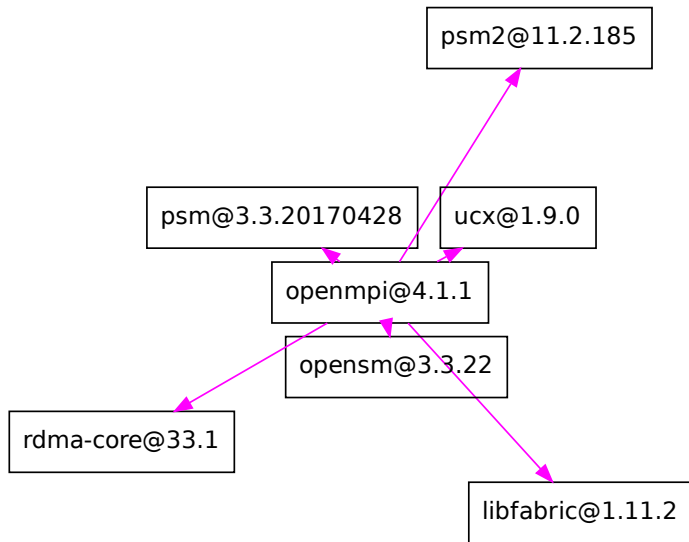
```
guix install mumps \  
  --with-input=scotch=pt-scotch
```

```
guix build chameleon \  
  --with-branch=starpu=master
```

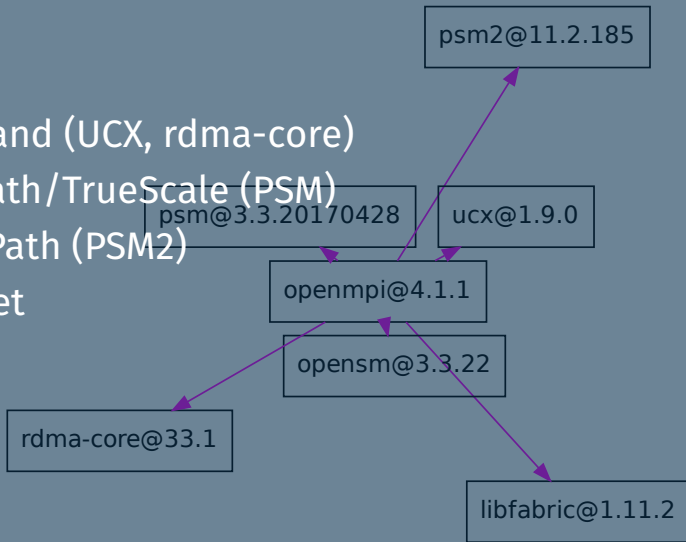
- ▶ `--with-commit`
- ▶ `--with-patch`
- ▶ `--with-input`
- ▶ `--with-c-toolchain`
- ▶ `--with-configure-flag`
- ▶ ...

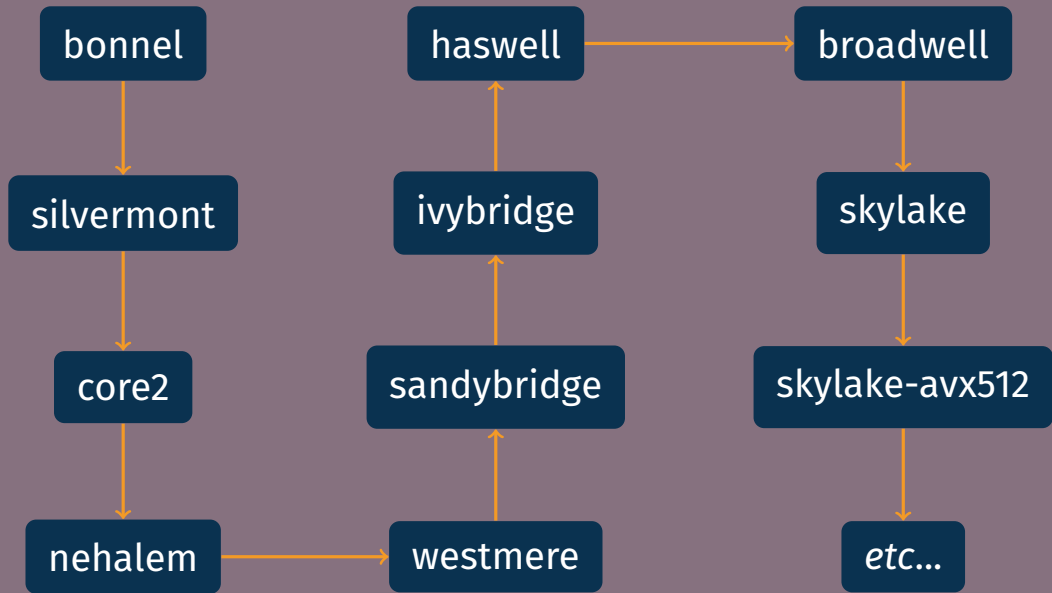
[https://guix.gnu.org/manual/devel/en/html_node/
Package-Transformation-Options.html](https://guix.gnu.org/manual/devel/en/html_node/Package-Transformation-Options.html)

3. Performance portability.



- ▶ InfiniBand (UCX, rdma-core)
- ▶ InfiniPath/TrueScale (PSM)
- ▶ Omni-Path (PSM2)
- ▶ Ethernet
- ▶ ...





```
$ spack spec netcdf-c
```

```
Concretized
```

```
-----  
netcdf-c@4.8.1... arch=linux-ubuntu18.04-skylake_avx512  
  ^hdf5@1.10.7... arch=linux-ubuntu18.04-skylake_avx512  
    ^cmake@3.21.4... arch=linux-ubuntu18.04-skylake_avx512  
      ^ncurses@6.2... arch=linux-ubuntu18.04-skylake_avx512  
        ^pkgconf@1.8.0... arch=linux-ubuntu18.04-skylake_avx512  
          ^openssl@1.1.1l... arch=linux-ubuntu18.04-skylake_avx512  
            ^perl@5.34.0... arch=linux-ubuntu18.04-skylake_avx512  
              ^berkeley-db@18.1.40... arch=linux-ubuntu18.04-skylake_avx512  
                ^bzip2@1.0.8... arch=linux-ubuntu18.04-skylake_avx512  
                  ^diffutils@3.8... arch=linux-ubuntu18.04-skylake_avx512  
                    ^libiconv@1.16... arch=linux-ubuntu18.04-skylake_avx512  
                      ^gdbm@1.19... arch=linux-ubuntu18.04-skylake_avx512  
                        ^readline@8.1... arch=linux-ubuntu18.04-skylake_avx512  
                          ^zlib@1.2.11... arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
```

```
Concretized
```

```
-----  
netcdf-c@4.8.1... arch=linux-ubuntu18.04-skylake_avx512  
  ^hdf5@1.10.7... arch=linux-ubuntu18.04-skylake_avx512  
    ^cmake@3.21.4... arch=linux-ubuntu18.04-skylake_avx512  
      ^ncurses@6.2... arch=linux-ubuntu18.04-skylake_avx512  
        ^pkgconf@1.8.0... arch=linux-ubuntu18.04-skylake_avx512  
          ^openssl@1.1.1l... arch=linux-ubuntu18.04-skylake_avx512  
            ^perl@5.34.0... arch=linux-ubuntu18.04-skylake_avx512  
              ^berkeley-db@18.1.40... arch=linux-ubuntu18.04-skylake_avx512  
                ^bzip2@1.0.8... arch=linux-ubuntu18.04-skylake_avx512  
                  ^diffutils@3.8... arch=linux-ubuntu18.04-skylake_avx512  
                    ^libiconv@1.16... arch=linux-ubuntu18.04-skylake_avx512  
                      ^gdbm@1.19... arch=linux-ubuntu18.04-skylake_avx512  
                        ^readline@8.1... arch=linux-ubuntu18.04-skylake_avx512  
                          ^zlib@1.2.11... arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
```

```
Concretized
```

```
-----  
netcdf-c@4.8.1... arch=linux-ubuntu18.04-skylake_avx512  
  ^hdf5@1.10.7... arch=linux-ubuntu18.04-skylake_avx512  
    ^cmake@3.21.4... arch=linux-ubuntu18.04-skylake_avx512  
      ^ncurses@6.2... arch=linux-ubuntu18.04-skylake_avx512  
        ^pkgconf@1.8.0... arch=linux-ubuntu18.04-skylake_avx512  
          ^openssl@1.1.1l... arch=linux-ubuntu18.04-skylake_avx512  
            ^perl@5.34.0... arch=linux-ubuntu18.04-skylake_avx512  
              ^berkeley-db@18.1.40... arch=linux-ubuntu18.04-skylake_avx512  
                ^bzip2@1.0.8... arch=linux-ubuntu18.04-skylake_avx512  
                  ^diffutils@3.8... arch=linux-ubuntu18.04-skylake_avx512  
                    ^libiconv@1.16... arch=linux-ubuntu18.04-skylake_avx512  
                      ^gdbm@1.19... arch=linux-ubuntu18.04-skylake_avx512  
                        ^readline@8.1... arch=linux-ubuntu18.04-skylake_avx512  
                          ^zlib@1.2.11... arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
```

```
Concretized
```

```
-----  
netcdf-c@4.8.1... arch=linux-ubuntu18.04-skylake_avx512  
  ^hdf5@1.10.7... arch=linux-ubuntu18.04-skylake_avx512  
    ^cmake@3.21.4... arch=linux-ubuntu18.04-skylake_avx512  
      ^ncurses@6.2... arch=linux-ubuntu18.04-skylake_avx512  
        ^pkgconf@1.8.0... arch=linux-ubuntu18.04-skylake_avx512  
          ^openssl@1.1.1l... arch=linux-ubuntu18.04-skylake_avx512  
            ^perl@5.34.0... arch=linux-ubuntu18.04-skylake_avx512  
              ^berkeley-db@18.1.40... arch=linux-ubuntu18.04-skylake_avx512  
                ^bzip2@1.0.8... arch=linux-ubuntu18.04-skylake_avx512  
                  ^diffutils@3.8... arch=linux-ubuntu18.04-skylake_avx512  
                    ^libiconv@1.16... arch=linux-ubuntu18.04-skylake_avx512  
                      ^gdbm@1.19... arch=linux-ubuntu18.04-skylake_avx512  
                        ^readline@8.1... arch=linux-ubuntu18.04-skylake_avx512  
                          ^zlib@1.2.11... arch=linux-ubuntu18.04-skylake_avx512  
https://spack.readthedocs.io/en/latest/getting\_started.html
```

```
$ spack spec netcdf-c
```

```
Concretized
```

```
-----  
netcdf-c@4.8.0
```

```
^hdf5@1.10.4
```

```
^cmake@3.18.2
```

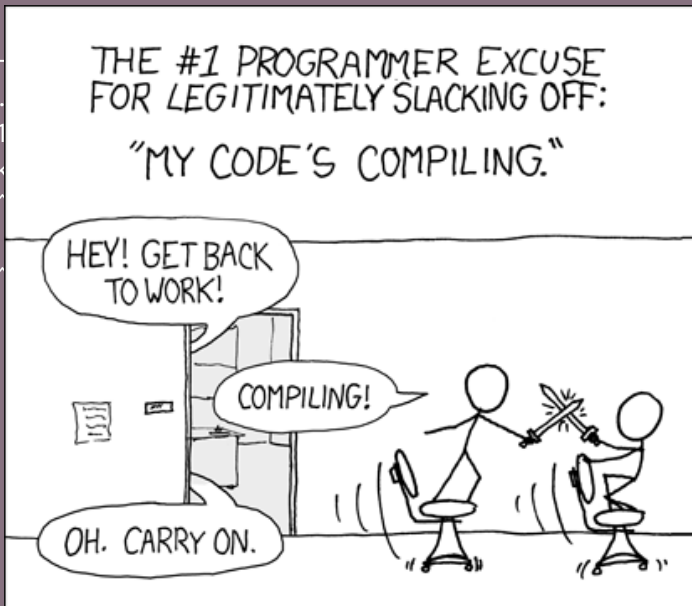
THE #1 PROGRAMMER EXCUSE
FOR LEGITIMATELY SLACKING OFF:

"MY CODE'S COMPILING."

HEY! GET BACK
TO WORK!

COMPILING!

OH. CARRY ON.



:512

lake_avx512

avx512

_avx512

lake_avx512

lake_avx512

lake_avx512

lake_avx512

lake_avx512

lake_avx512

lake_avx512

GNU libc

Libgcrypt

Nettle

OpenBLAS

BLIS

FFTW

GMP

Julia

Rust

<https://hpc.guix.info/blog/2018/01/pre-built-binaries-vs-performance/>

```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)
```

```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)
```

**Package
multi-versioning**

```
$ guix shell --tune eigen-benchmarks -- \
    benchBlasGemm 240 240 240
guix shell: tuning for CPU micro-architecture skylake
240 x 240 x 240
cblas: 0.203131 (16.333 GFlops/s)
eigen : 0.0929638 (35.688 GFlops/s)
```

<https://hpc.guix.info/blog/2022/01/tuning-packages-for-a-cpu-micro-architecture/>

4. Interoperability.

```
$ guix pack \  
    python python-numpy python-scipy  
...  
/gnu/store/...-pack.tar.gz
```

```
$ guix pack --relocatable \  
python python-numpy python-scipy  
...  
/gnu/store/...-pack.tar.gz
```

<https://hpc.guix.info/blog/2020/05/faster-relocatable-packs-with-fakechroot/>

```
$ guix pack --format=squashfs \  
    python python-numpy python-scipy  
...  
/gnu/store/...-singularity-image.tar.gz
```

```
$ guix pack --format=docker \  
python python-numpy python-scipy  
...  
/gnu/store/...-docker-image.tar.gz
```



ENVIRONMENT
MODULES

```
guix module create -o /opt/modules \  
gcc-toolchain openmpi netcdf gromacs
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

```
guix module create -o /opt/modules \  
  --tune=skylake-avx512 \  
  gcc-toolchain openmpi netcdf gromacs
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

```
guix module create -o /opt/modules \  
  --manifest=manifest.scm
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

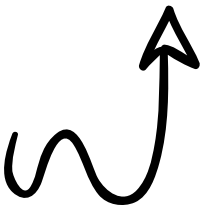
5. Open science & reproducible research.



Software Heritage



The Re**Science** Journal



<https://guix.gnu.org/en/blog/2019/connecting-reproducible-deployment-to-a-long-term-source-code-archive/>

- ▶ P. Swartvagher, *On the Interactions between HPC Task-based Runtime Systems and Communication Libraries*, PhD thesis, Dec. 2022
- ▶ M. Felšöci, *Fast Solvers for High-Frequency Aeroacoustics*, PhD thesis, Feb. 2023
- ▶ N. Vallet et al., *Toward practical transparent verifiable and long-term reproducible research using Guix*, Nature Scientific Data, Oct. 2022

Wrapping up.

- 1. robustness**
- 2. flexibility**
- 3. performance portability**
- 4. interoperability**
- 5. reproducible research**



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



`ludovic.courtes@inria.fr | @civodul@toot.aquilenet.fr`

<https://hpc.guix.info>

Bonus slides!

```
$ guix build hwloc
```

isolated build: chroot, separate name spaces, etc.

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

hash of **all** the dependencies



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

```
$ guix gc --references /gnu/store/...-hwloc-1.11.2  
/gnu/store/...-glibc-2.33  
/gnu/store/...-gcc-10.3.0-lib  
/gnu/store/...-hwloc-2.9.0
```

```
$ guix build hwloc
```

```
/gnu/store/h2g4sf72...-hwloc-1.11.2
```

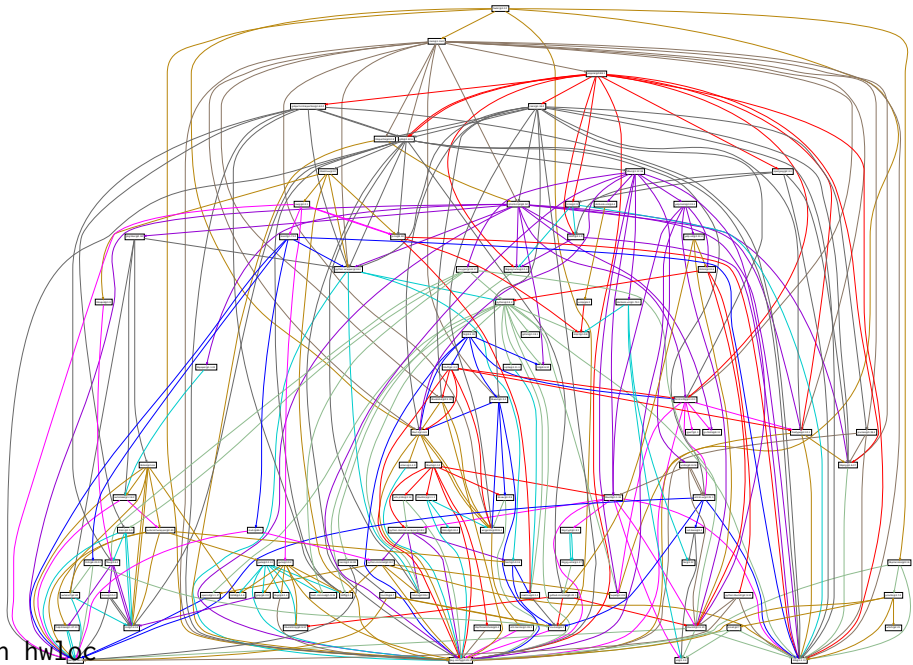
```
$ guix gc --references /gnu/store/...-hwloc-1.11.2
```

```
/gnu/store/...-glibc-2.33
```

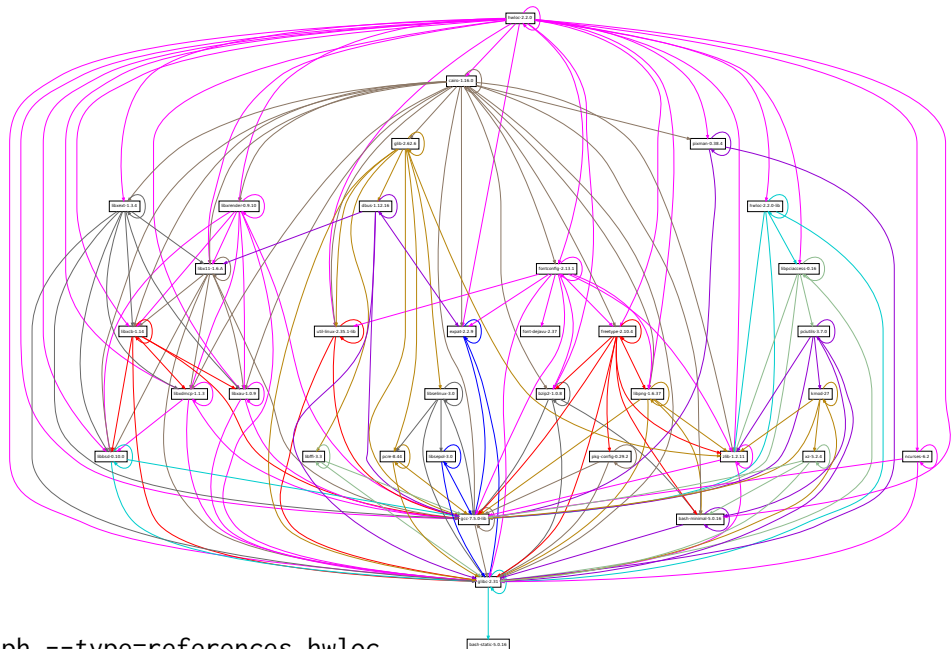
```
/gnu/store/...-gcc-10.3.0-lib
```

```
/gnu/store/...-hwloc-2.9.0
```

(nearly) bit-identical for everyone



guix graph hwloc



`guix graph --type=references hwloc`

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GNU Guix logo, CC-BY-SA 4.0, <https://gnu.org/s/guix/graphics>.

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