Reproducible environments with Guix

or how to be able to run your current code in ~5 years

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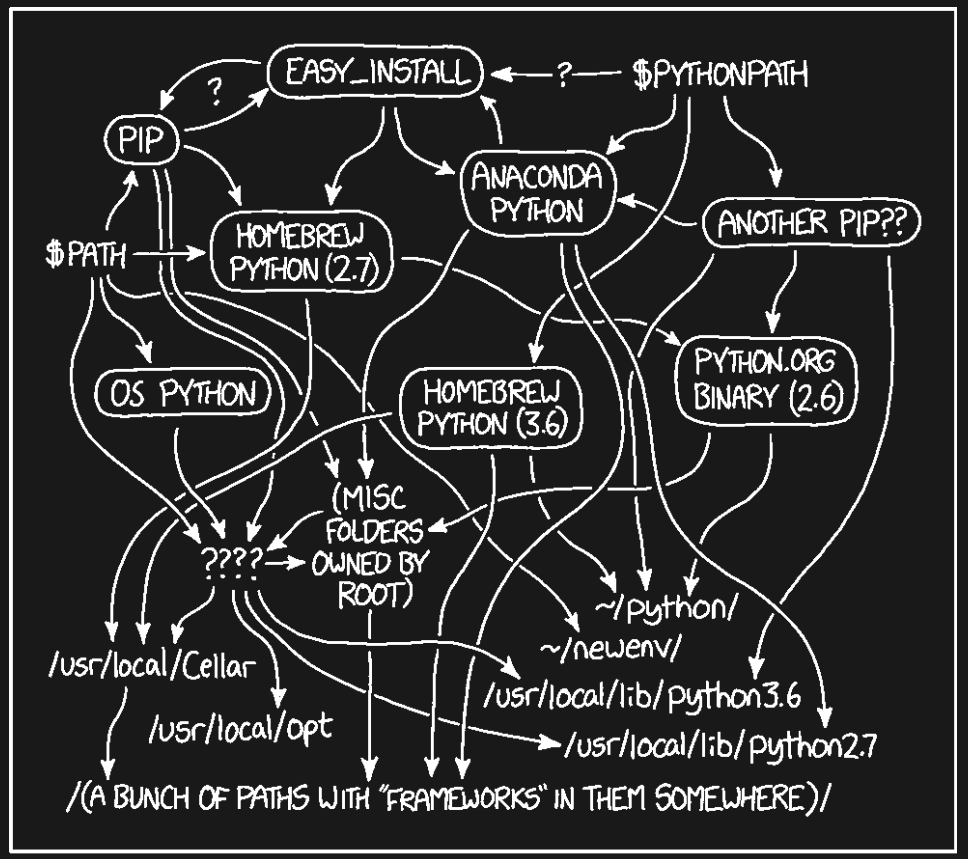
(MPE)



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

xkcd #1987 (30.04.2018)

2023-11-13, USM Code Coffee

Functional package management

What's it?

1. Install a package

```
$ guix install firefox
$ apt install firefox
```

2. Delete a package

```
$ guix remove firefox
$ apt remove firefox
```

3. Update database

```
$ guix pull
$ apt update
```

4. Undo

```
$ guix package --roll-back
$ apt 🤷🤷🤷
```

GNU Guix is a

- functional

  (package contents explicitly depend on its dependencies and *isolated* build environment)
- transactional

  (if something does wrong during the upgrade, the system just remains in its original state)
- source-based

  (everything is built from source, but in most cases binary substitutes are used)

package manager with particular focus on *reproducibility*.

```
$ guix install samtools bowtie
```

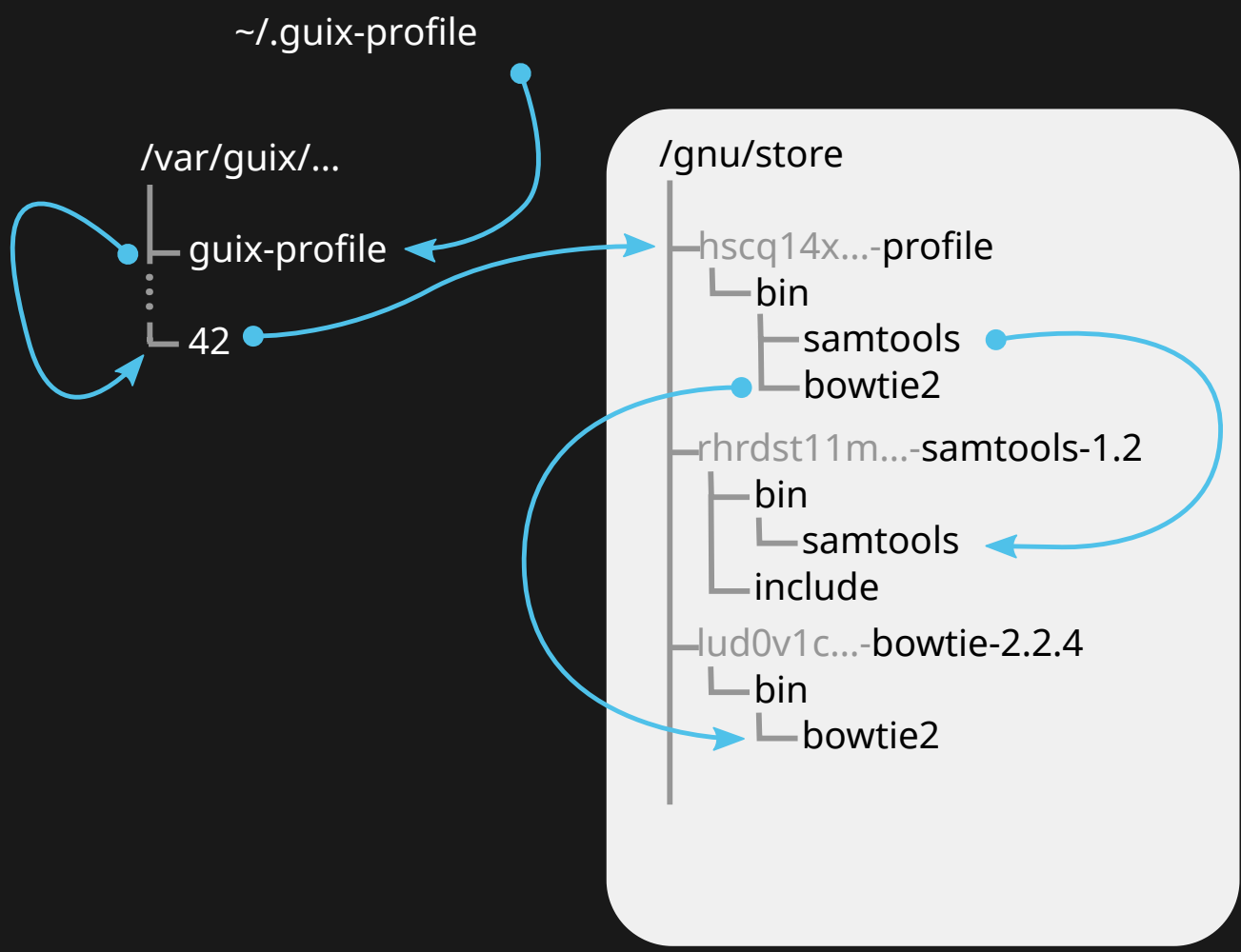


Figure stolen from C. Baines slides who in turn gives credit to Ricardo Wurmus

```
$ guix remove bowtie
```

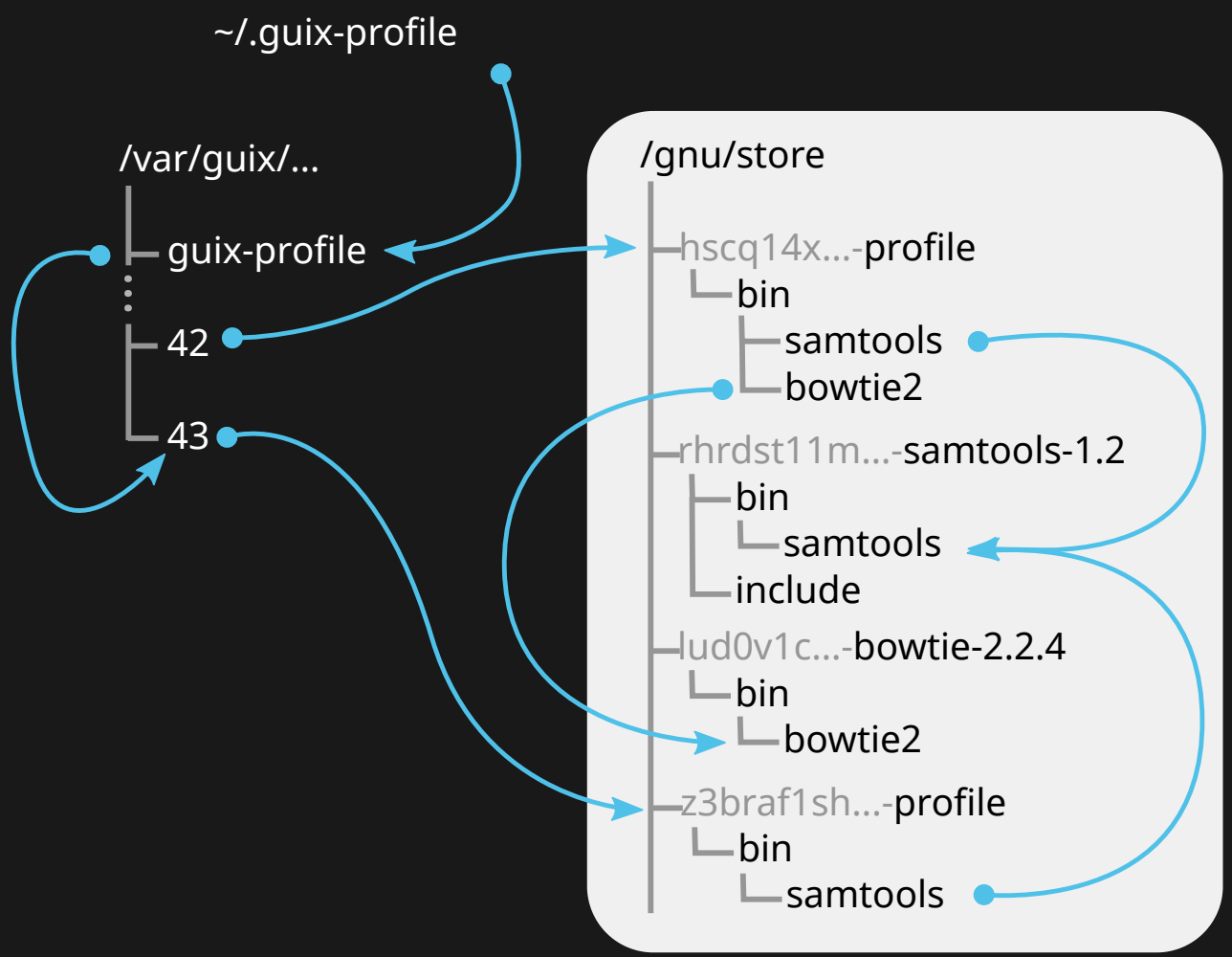
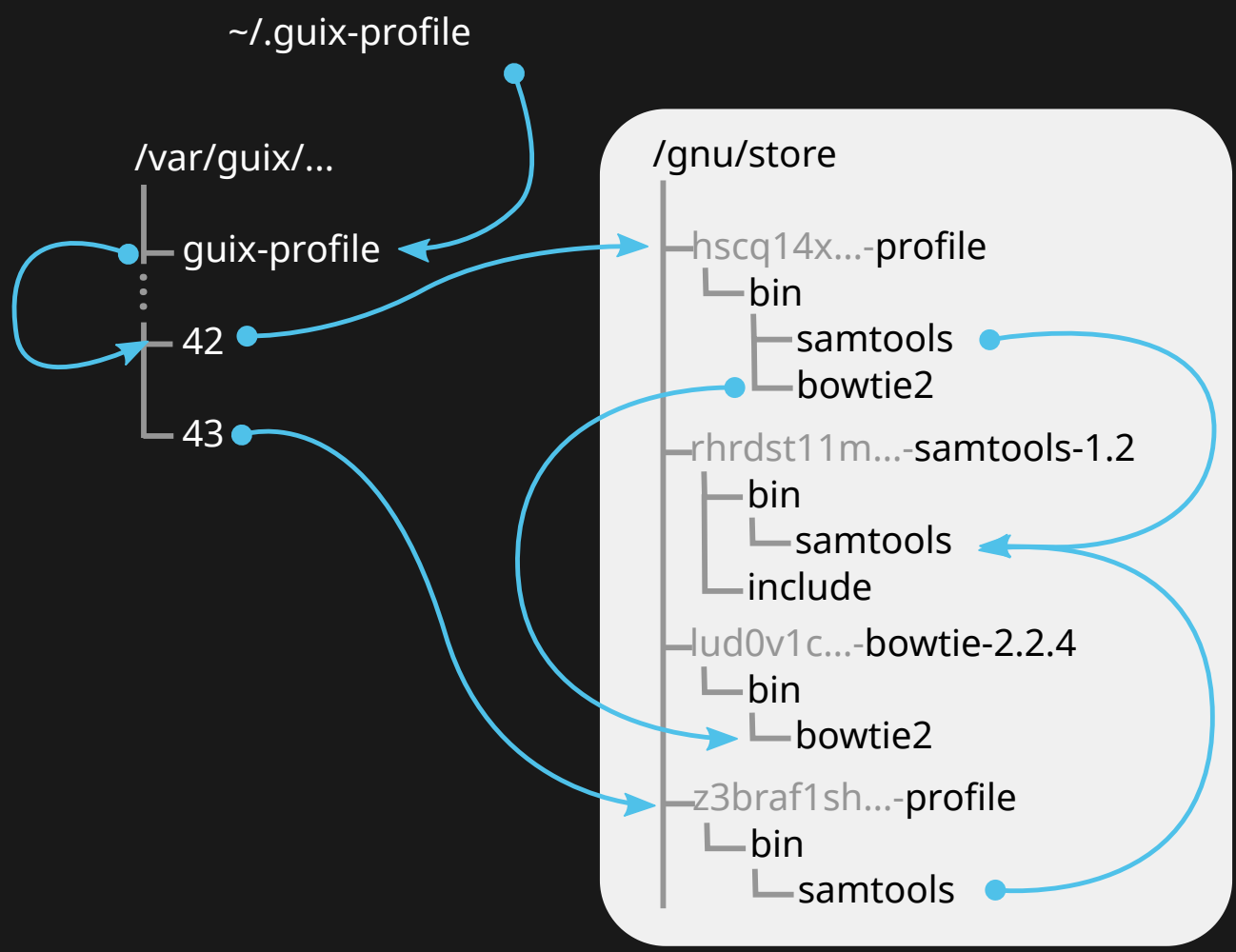


Figure stolen from C. Baines slides who in turn gives credit to Ricardo Wurmus

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



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Managing computational environments

0. pip and virtualenv

1. Manages python dependencies
2. Does not ensure compatibility of dependencies (just installs them)
3. Makes assumptions about outside environment (python, C/C++/Fortran libraries)

An example

```
$ pip install scipy
 ... lots of errors ...
 numpy.distutils.system_info.NotFoundError: No BLAS/LAPACK libraries
found. Note: Accelerate is no longer supported.
  To build Scipy from sources, BLAS & LAPACK libraries need to be
installed.
  See site.cfg.example in the Scipy source directory and
  https://docs.scipy.org/doc/scipy/reference/building/index.html for
details.
  ----------------------------------------
```

1/2. environment modules

```
$ module purge
$ module load intel/19.1.3 impi/2019.9 mkl/2019.4 \
         anaconda/3/2021.11 cmake/3.24 hdf5-mpi/1.12.1
```

1. Adjusts environment variables (PATH etc) to make additional software available.
2. Consistency of dependencies – ensured ‘by hand’

`find-module hdf5-mpi | grep 1.14.2` on cobra.mpcdf.mpg.de

```
hdf5-mpi/1.14.1 (after loading gcc/10 impi/2021.6) hdf5-mpi/1.14.1 (after loading gcc/10 impi/2021.7)
hdf5-mpi/1.14.1 (after loading gcc/10 impi/2021.9) hdf5-mpi/1.14.1 (after loading gcc/10 openmpi/4)
hdf5-mpi/1.14.1 (after loading gcc/10 openmpi/4.1) hdf5-mpi/1.14.1 (after loading gcc/11 impi/2021.6)
hdf5-mpi/1.14.1 (after loading gcc/11 impi/2021.7) hdf5-mpi/1.14.1 (after loading gcc/11 impi/2021.9)
hdf5-mpi/1.14.1 (after loading gcc/11 openmpi/4)   hdf5-mpi/1.14.1 (after loading gcc/11 openmpi/4.1)
hdf5-mpi/1.14.1 (after loading gcc/12 impi/2021.6) hdf5-mpi/1.14.1 (after loading gcc/12 impi/2021.7)
hdf5-mpi/1.14.1 (after loading gcc/12 impi/2021.9) hdf5-mpi/1.14.1 (after loading gcc/12 openmpi/4)
hdf5-mpi/1.14.1 (after loading gcc/12 openmpi/4.1) hdf5-mpi/1.14.1 (after loading gcc/13 impi/2021.6)
hdf5-mpi/1.14.1 (after loading gcc/13 impi/2021.7) hdf5-mpi/1.14.1 (after loading gcc/13 impi/2021.9)
hdf5-mpi/1.14.1 (after loading gcc/13 openmpi/4)   hdf5-mpi/1.14.1 (after loading gcc/13 openmpi/4.1)
hdf5-mpi/1.14.1 (after loading intel/2023.1.0.x impi/2021.9) hdf5-mpi/1.14.1 (after loading intel/2023.1.0.x openmpi/4)
hdf5-mpi/1.14.1 (after loading intel/2023.1.0.x openmpi/4.1) hdf5-mpi/1.14.1 (after loading intel/21.6.0 impi/2021.6)
hdf5-mpi/1.14.1 (after loading intel/21.6.0 openmpi/4)   hdf5-mpi/1.14.1 (after loading intel/21.6.0 openmpi/4.1)
hdf5-mpi/1.14.1 (after loading intel/21.7.1 impi/2021.7) hdf5-mpi/1.14.1 (after loading intel/21.7.1 openmpi/4)
hdf5-mpi/1.14.1 (after loading intel/21.7.1 openmpi/4.1)
```

… but what if I need `hdf5-mpi/1.14` and `intel/19`?

1. conda (or mamba)

1. Manages *packages* (not limited to python)
2. Solves entire *environments*

```
$ conda create -n test astropy

The following packages will be downloaded:
    package                    |            build
    ---------------------------|-----------------
    ...
    astropy-5.3.4              |  py312ha883a20_0         8.8 MB
    blas-1.0                   |              mkl           6 KB
    bzip2-1.0.8                |       h7b6447c_0          78 KB
    ...
------------------------------------------------------------
                                           Total:       269.6 MB
```

1. conda (or mamba) – hidden assumptions

1. Manages *binaries* [1]:
   - compiler versions?
   - architecture-specific optimizations?
2. `ldd $HOME/opt/micromamba/envs/…/bin/gfortran`

```
linux-vdso.so.1 (0×00007ffcf874f000)
libm.so.6 ⇒ /lib/x86_64-linux-gnu/libm.so.6 (0×00007f7058af8000)
libc.so.6 ⇒ /lib/x86_64-linux-gnu/libc.so.6 (0×00007f7058906000)
/lib64/ld-linux-x86-64.so.2 (0×00007f7058c6b000)
```

… still depends on the underlying system

1. However, see conda-forge and feedstocks

2. Docker or Apptainer

1. Manages self-contained *images*
2. Builds *isolated* (using Linux kernel features) environments
3. Environments are immutable, but can be extended

Example (non-scientific..)

```
$ docker run --name … -e POSTGRES_PASSWORD=… -d postgres
Unable to find image 'postgres:latest' locally
latest: Pulling from library/postgres
578acb154839: Downloading
[==========================================>    ]  27.28MB/29.15MB
8a9a8dd839ec: Download complete
9a28d48e5d8f: Download complete
…
```

Dockerfiles (and reproducibility)

slothai/numpy does not use apk update (i.e. a dependency on a remote resource), but some Dockerfiles do

```
 1  FROM slothai/openblas as openblas
 2  FROM python:3.6.5-alpine3.7
 3  # Metadata as defined at http://label-schema.org
 4  ARG BUILD_DATE
 5  ARG VCS_REF
 6  ARG NUMPY_VERSION=1.14.3
 7
 8  COPY --from=openblas /opt/OpenBLAS/ /opt/OpenBLAS/
 9  LABEL org.label-schema.build-date=$BUILD_DATE \
10      org.label-schema.name="NumPy" \
11      org.label-schema.vcs-ref=$VCS_REF \
12      org.label-schema.vcs-url="https://github.com/slothai/docker-numpy" \
13      org.label-schema.vendor="SlothAI <https://slothai.github.io/>" \
14      org.label-schema.schema-version="1.0"
15  RUN apk add --no-cache --virtual .meta-build-dependencies \
16          gcc \
17          musl-dev && \
18      apk add --no-cache gfortran && \
19      wget -O numpy.tar.gz "https://github.com/numpy/numpy/archive/v$NUMPY_VERSION.tar.gz" && \
20      tar xzf numpy.tar.gz && rm -f numpy.tar.gz && \
21      echo -e "[openblas]\nlibraries = openblas\n\
22  library_dirs = /opt/OpenBLAS/lib\n\
23  include_dirs = /opt/OpenBLAS/include\n\
24  runtime_library_dirs = /opt/OpenBLAS/lib\
25  " > /numpy-$NUMPY_VERSION/site.cfg && \
26      pip install Cython==0.28.2 && \
27      cd /numpy-$NUMPY_VERSION/ && python setup.py build --parallel=$(nproc) --fcompiler=gfortran && \
28      python setup.py install && cd / && \
29      rm -rf /numpy-$NUMPY_VERSION/ && \
30      pip uninstall --yes Cython && \
31      apk del .meta-build-dependencies && \
32      find / -type d -name __pycache__ -exec rm -r {} +
```

Guix Examples

Creating an environment

Declaring everything at once (manifests)

```
(specifications→manifest
  (list "openblas" "openmpi"
        ;; …
        "gcc-toolchain"))
```

and then

```
$ guix shell -m manifest.scm strace
                            #^^^^ additional package for debugging
```

Adding packages iteratively (profiles)

```
$ guix install openblas -p ./myenv
$ guix install openmpi -p ./myenv
$ guix package --export-manifest -p ./myenv > manifest.scm
```

Running code in the environment

```
$ guix shell -m manifest.scm
```

Pure environments

```
$ guix shell --pure --preserve=^OMP_NUM_THREADS …
```

unsets all environment variables (`PATH` and friends) except those that are `--preserve`d.

Containers

```
$ guix shell --container \
  --share=output-dir \
  --expose=…=/input-dir \
  -m manifest.scm \
  coreutils strace grep sed -- ./run -i /input-dir -o output-dir
```

process, filesystem (unless `--exposed` or `--shared`) and network isolation (unless `-N` is used) using Linux cgroups & namespaces.

< manifest for the current project >

Reproducing environments

What we need

1. Code and data
2. `manifest.scm`
3. A description the current Guix and used channels:

```
guix describe -f channels > guix-version-for-reproduction.txt
```

How to reproduce

```
guix time-machine -C guix-version-for-reproduction.txt -- shell -C ...
```

< code from 2021 example >

Missing software?

Custom channels

- E.g. https://github.com/guix-science/guix-science

```
;; add to ~/.config/guix/channels.scm
(channel
  (name 'guix-science)
  (url "https://github.com/guix-science/guix-science.git")
  (introduction
   (make-channel-introduction
        "b1fe5aaff3ab48e798a4cce02f0212bc91f423dc"
        (openpgp-fingerprint
         "CA4F 8CF4 37D7 478F DA05  5FD4 4213 7701 1A37 8446"))))
```

Import from another PM

```
$ guix import … >> /path/to/custom/definitions/file.scm
$ guix shell -L /path/to/custom/definitions …
```

Caveats

- Guix does not natively work on MacOS (but can work on a Linux VM inside)
- Requires root for installation, not available on an average HPC cluster (but there is `guix pack`);
- There is a lot of software still missing / outdated;
- Not as easy and fast as `conda install`;
- Scheme for writing packages / manifests;
- Build farm (ci.guix.gnu.org) sometimes fails to build everything in time and Guix starts building packages, which can take a while (use `guix weather …` to check);
- `/gnu/store` can weight a few hundred of gigabytes (but there is `guix gc` to clean currently unused package versions).

Links

- Nix, another functional package manager with similar features.
- Guix official documentation and blog.
- A community package search in non-official channels.
- Reproducible Software Environments in HPC workshop webpage with slides and recordings.
- What's in a package, a (bit sad) story about conda, nix, spack, guix and packaging `pytorch`
- "Toward practical transparent verifiable and long-term reproducible research using Guix", a paper in Nature Scientific Data.
- https://www.cbaines.net/projects/guix/freenode-live-2017/presentation
- Revealjs version of this presentation

Questions?