reproducible and user-controlled software management in HPC

with GNU Guix

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System Admins

prefer **mature** software, no variants, only apply unavoidable updates

use **stable** software for **systems**

Users

want **fresh** software, multiple variants, latest tools, **flexibility**

manage **user software** stack on their own

ad-hoc

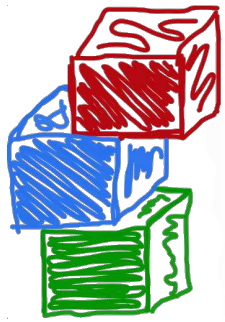
There is no way to **reproduce** the environment, even on the same machine at a different point in time.

volatile

Due to a **lack of isolation**, the environment will change or even break when the host system changes.

primitive

No safe upgrades or **roll-backs**.
No separation for different workflows.
Unportable.



easybuild

CONDA

Spack

Installing software is easy now!

...but reproducibility is still out of reach

Open **boegel** opened this issue on Nov 5, 2013 · 0 comments

boegel commented on Nov 5, 2013 — Member

It *seems* like the GCC libraries (e.g. `libiberty.a`) sometimes end up being built with `-fPIC` (e.g. on SL5), and sometimes not (e.g. on SL6), while `eb` is performing the exact same build procedure.

This causes problems for `cairo` (see) and `ExtraE` (part of UNITE), which require `libiberty.a` to be built with `-fPIC`. The `cairo` builds works fine on SL5, but doesn't work on `SL6` (see also hpcugent/easybuild-easyconfigs#494 (comment)).

Installing software is easy now!

...but reproducibility is still out of reach

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
```

seibert commented on May 13, 2015

There can be non-trivial issues with glibc that make it hard to distribute truly portable packages. I've been in situations where I couldn't easily deal with the range of Linux distributions that my colleagues were using.

After activating an environment `libselinux.so.1: cannot open shared object file` #5640

Open **Nagasaki45** opened this issue 16 days ago · 1 comment

Nagasaki45 commented 16 days ago • edited

I have an `environment.yml` file as pasted bellow. When I create an environment from it, and activate it, I see some weird bugs:

```
(myenv) $ vim
vim: error while loading shared libraries: libselinux.so.1: cannot open shared object file: N

(myenv) $ /bin/pytho
Could not find plat
Could not find plat
Consider setting $P
Fatal Python error:
ModuleNotFoundError

Current thread 0x00
[1]    7891 abort (
```

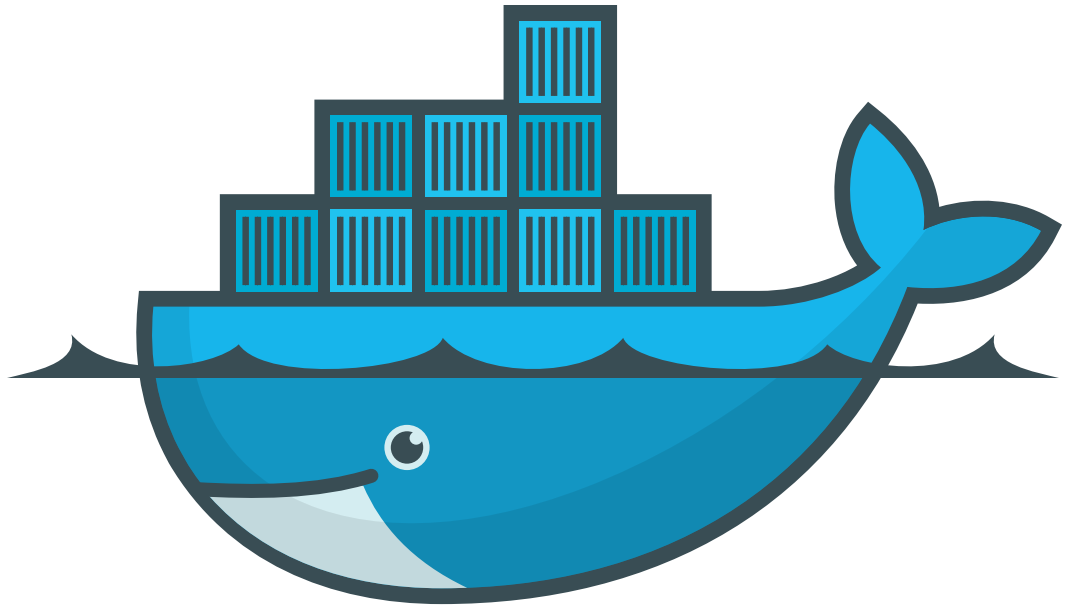
libgfortran broken? #686

Open **swryan** opened this issue on Mar 7, 2016 · 35 comments

swryan commented on Mar 7, 2016

Started getting this error a couple days ago:

`ImportError: /home/travis/miniconda/lib/python2.7/site-packages/scipy/special/../../../../libgfortran.so.3: version` GFORTRAN_1.4' not found (required by /usr/lib/liblapack.so.3gf)`



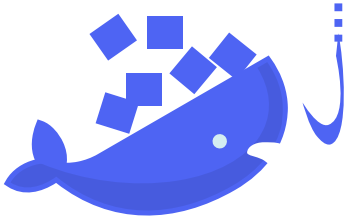
docker

100% reproducible
We have all the bits!

100% reproducible
We have all the bits!

100% stateful
We only have the bits!

App bundles are convenient



lack means of abstraction

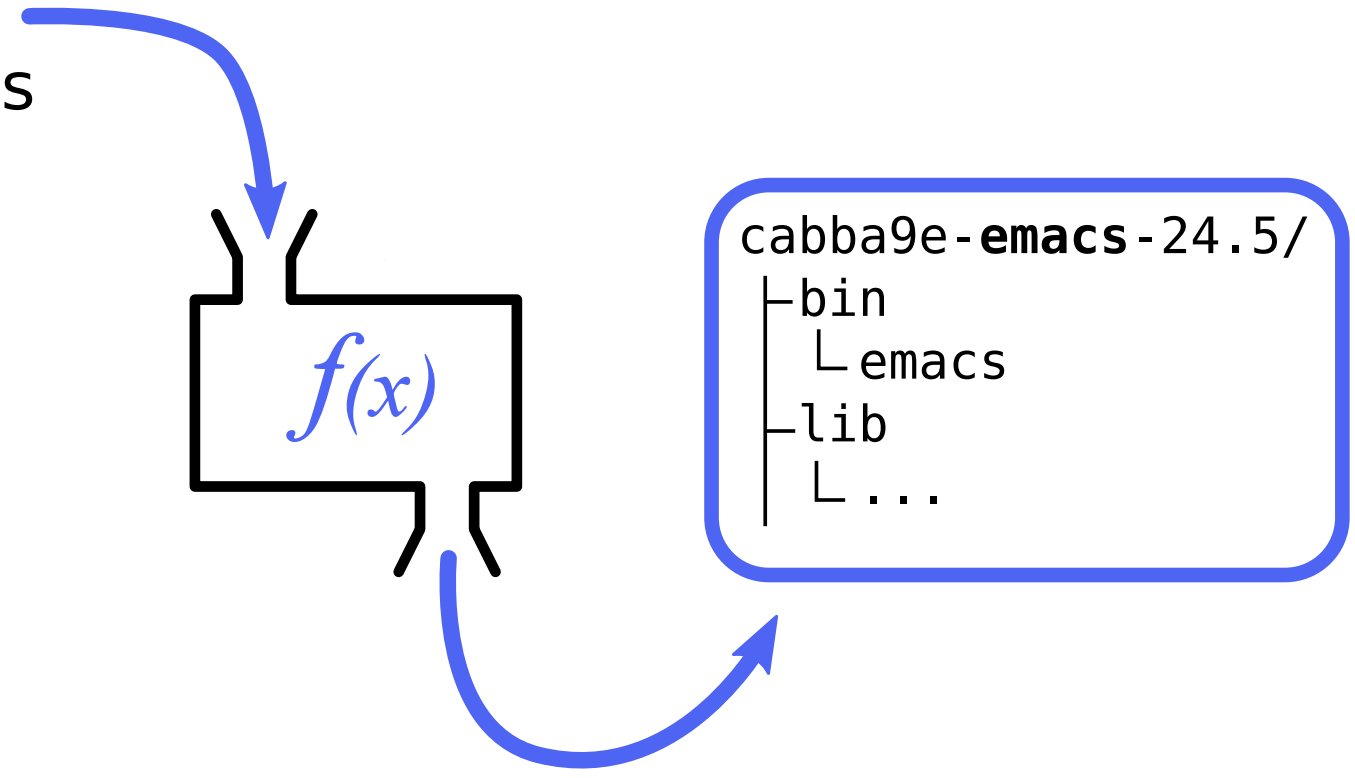
don't compose well

are like giant statically linked binaries


Guix

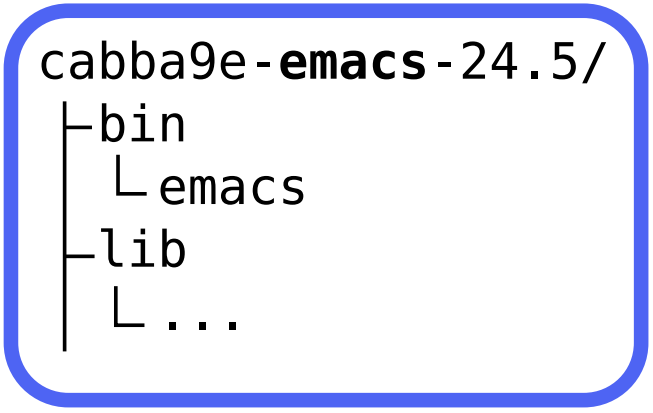
Functional packaging

headers
sources
build tools
libraries
...

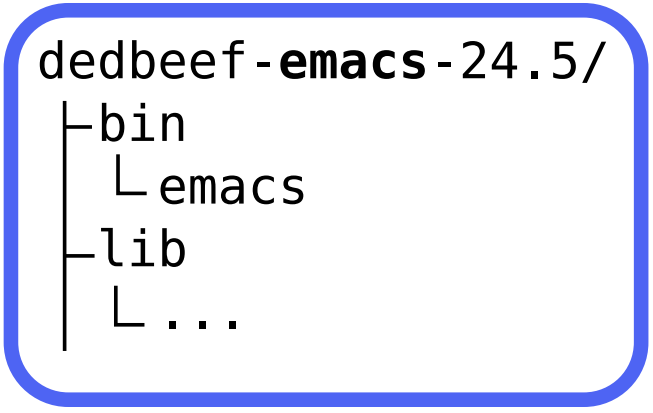


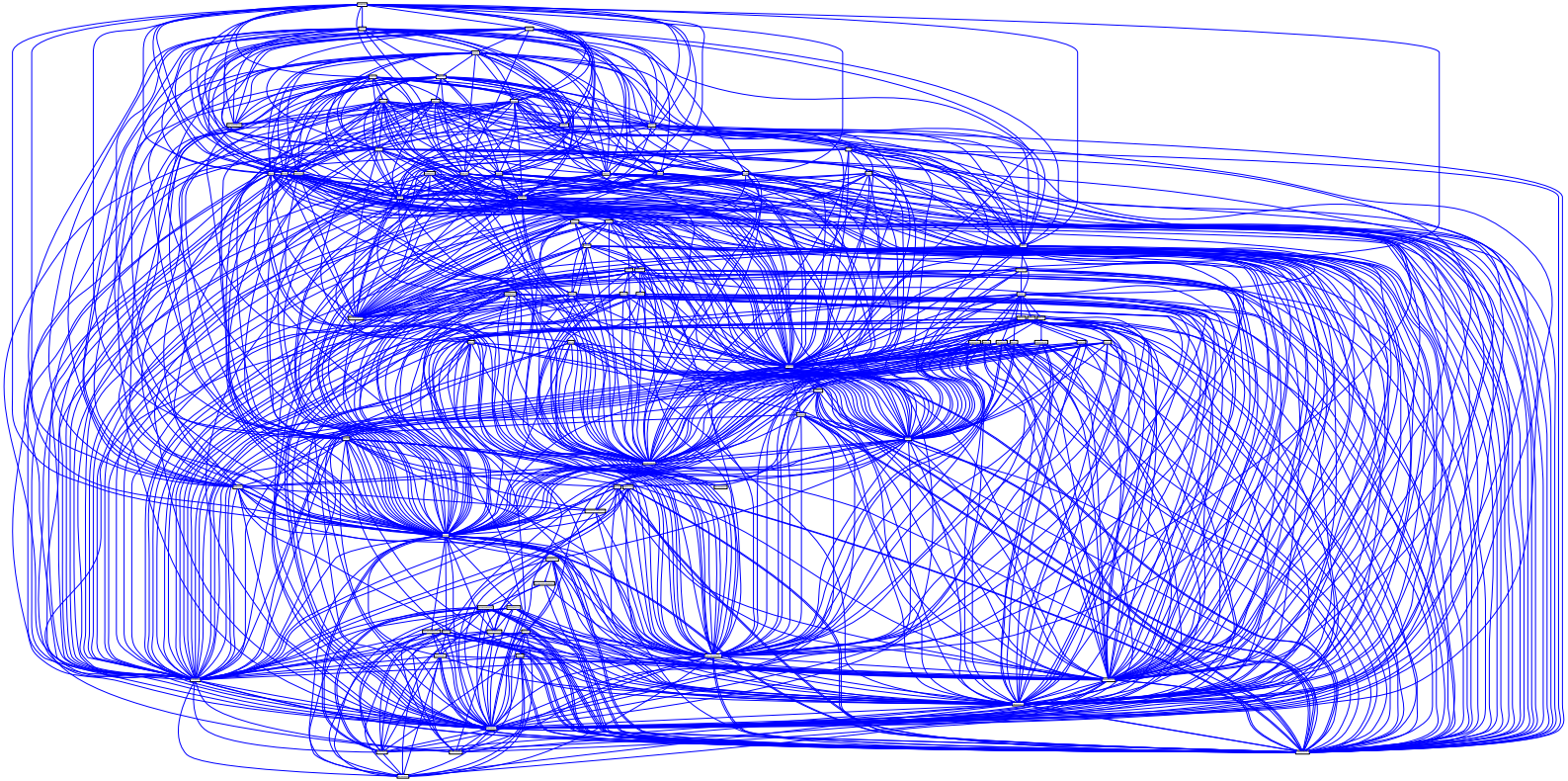
Functional packaging

Same inputs?
Same output!



Different inputs?
Different outputs.





```
guix gc --references
    /gnu/store/…-foo-0.9
```

```
/gnu/store/…-glibc-2.25
/gnu/store/…-gcc-4.9.3-lib
/gnu/store/…-bar-0.7b
/gnu/store/…-baz-1.4.9
/gnu/store/…-foo-0.9
```

```
guix package -i baz
     --with-input=foo=bar
```

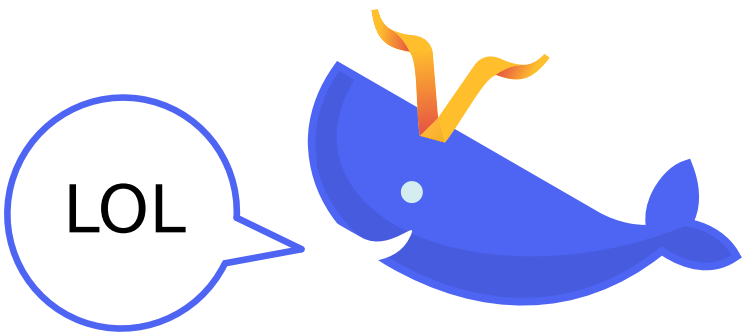
```
guix package -i baz
     --with-source=baz-1.0.tgz
```

guix pack samtools bedtools

/gnu/store/…-pack.tar.gz

guix pack -f **docker** samtools bedtools

/gnu/store/
…-docker-pack.tar.gz



guix package --**manifest**=GeneNetwork

All you need is:

Guix version + package manifest

(+ source code)

1. The level of abstraction matters
2. Guix enables reproducible and safe experimentation
3. Guix makes environment sharing easy
4. Joint Guix HPC project started this week

Join us!

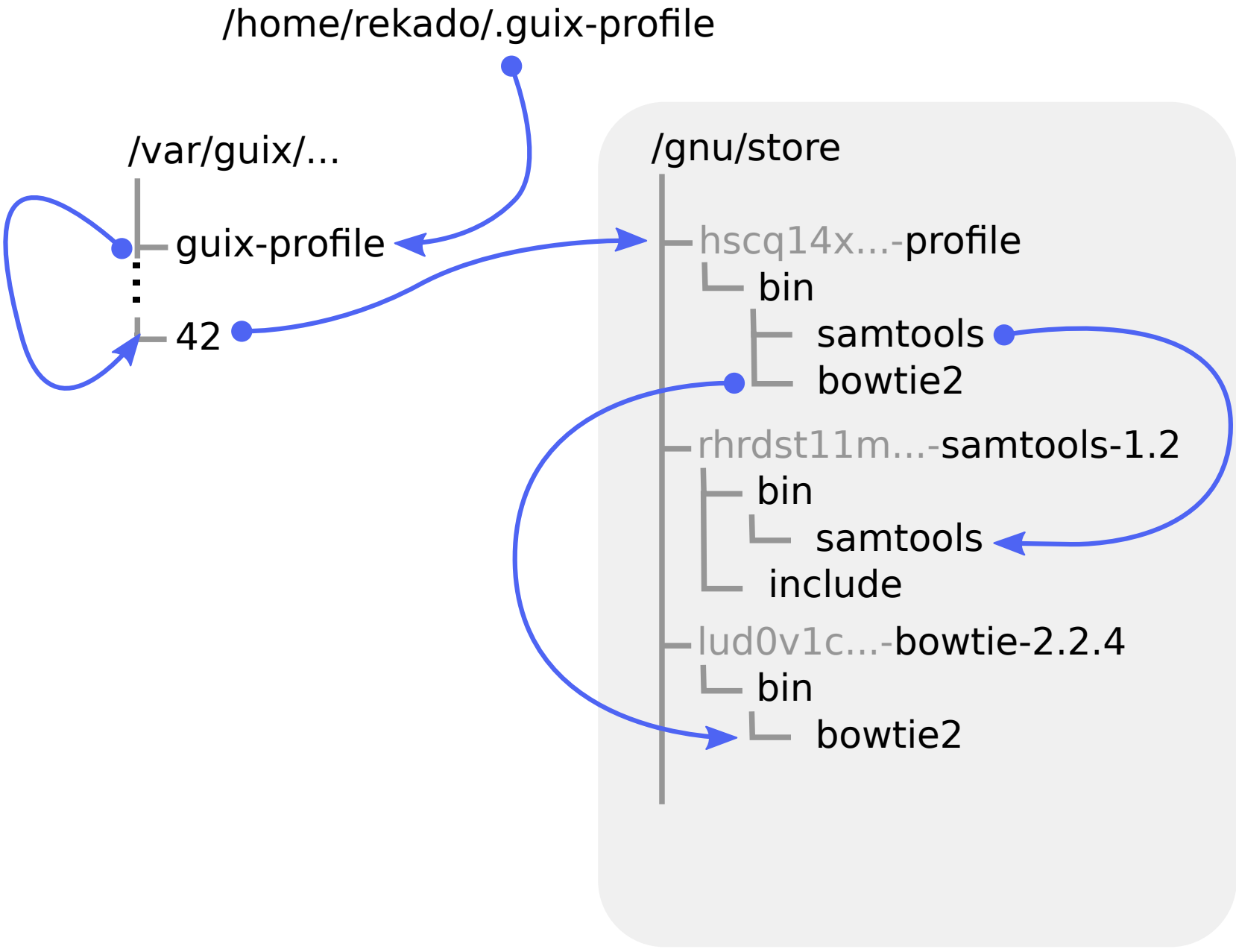
#guix on irc.freenode.net

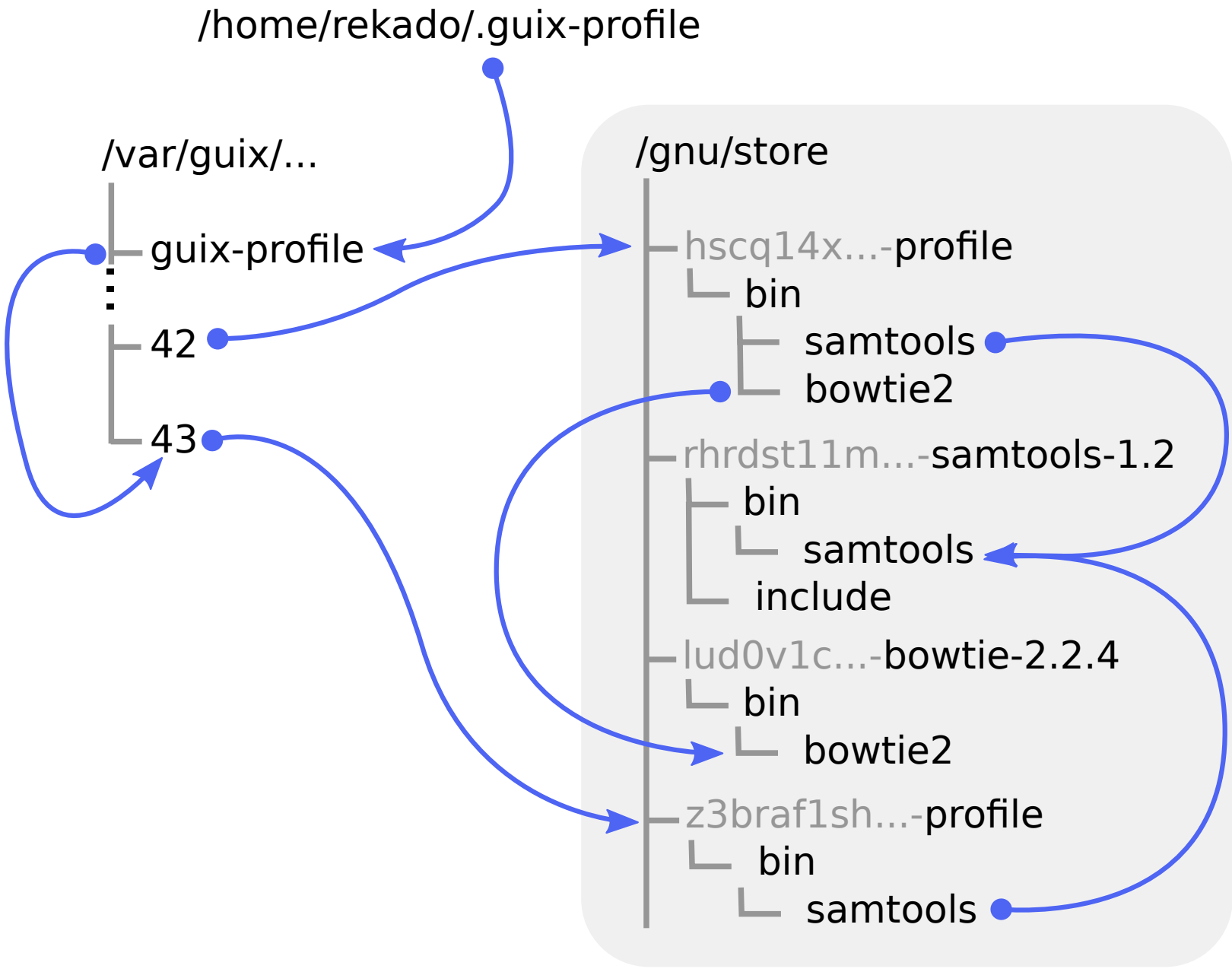
https://gnu.org/s/guix

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

ricardo.wurmus@mdc-berlin.de

guix-hpc@gnu.org


/home/rekado/.guix-profile
/var/guix/...
guix-profile
42
/gnu/store
hscq14x...-profile
bin
samtools
bowtie2
rhrdst11m...-samtools-1.2
bin
samtools
include
lud0v1c...-bowtie-2.2.4
bin
bowtie2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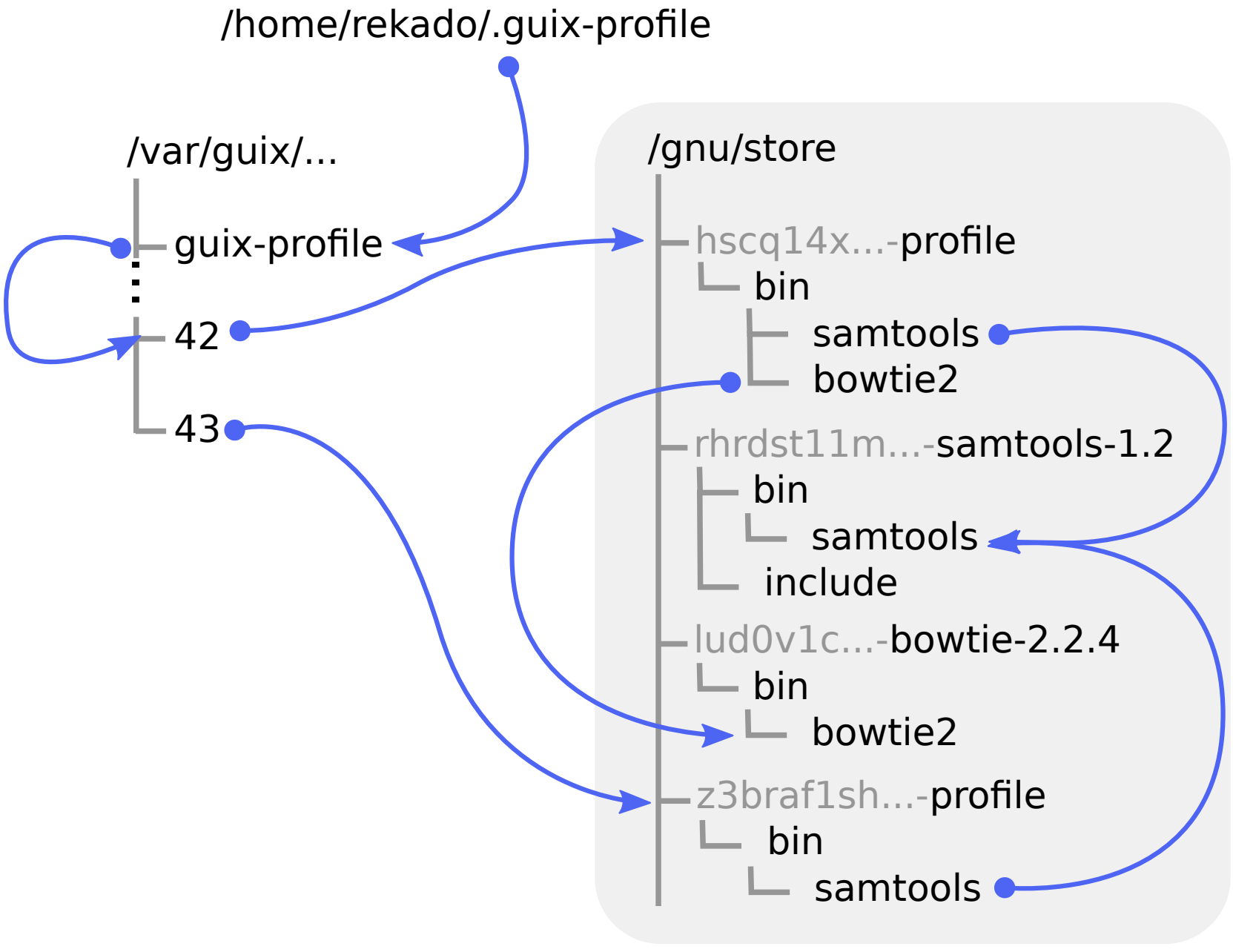
samtools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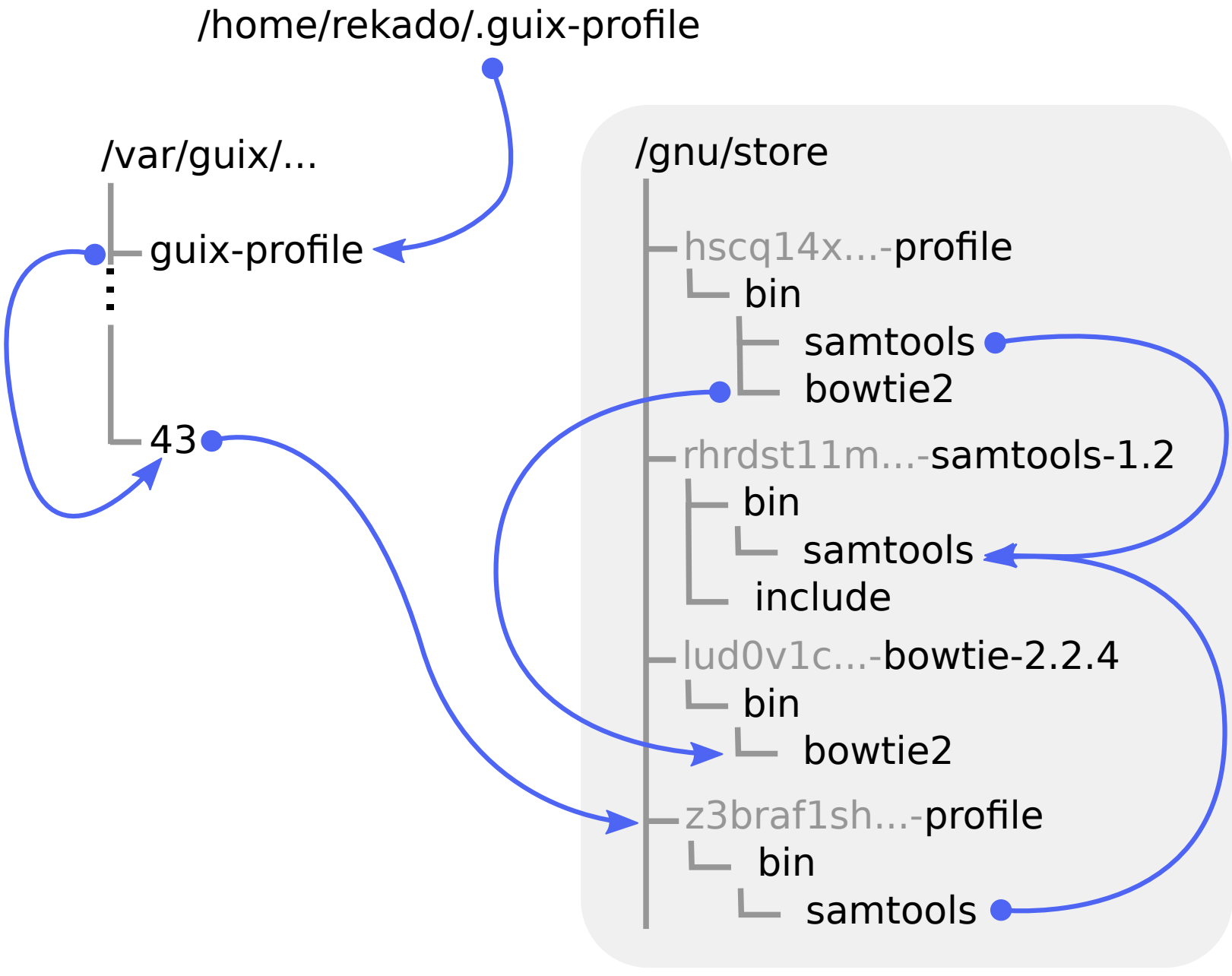
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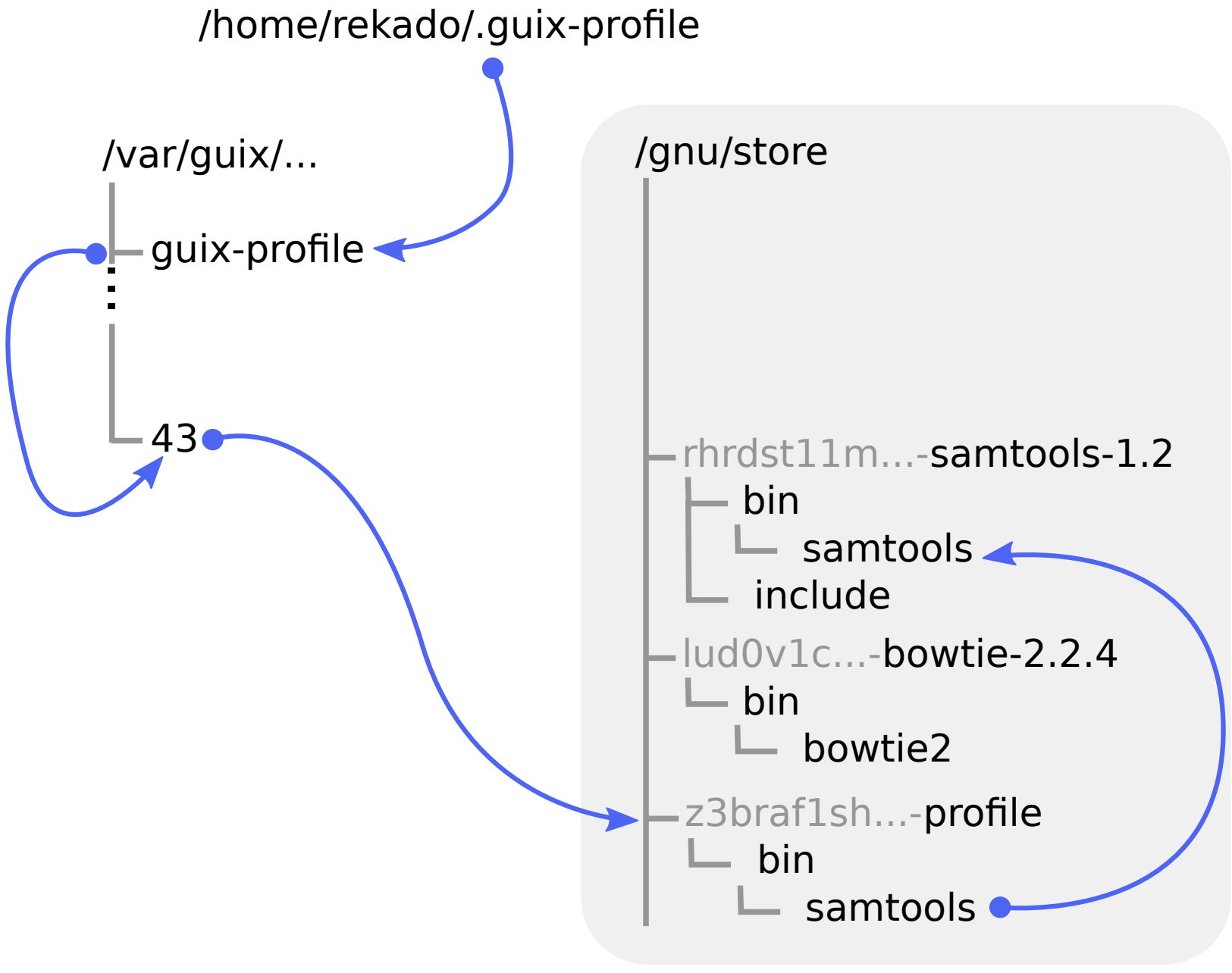
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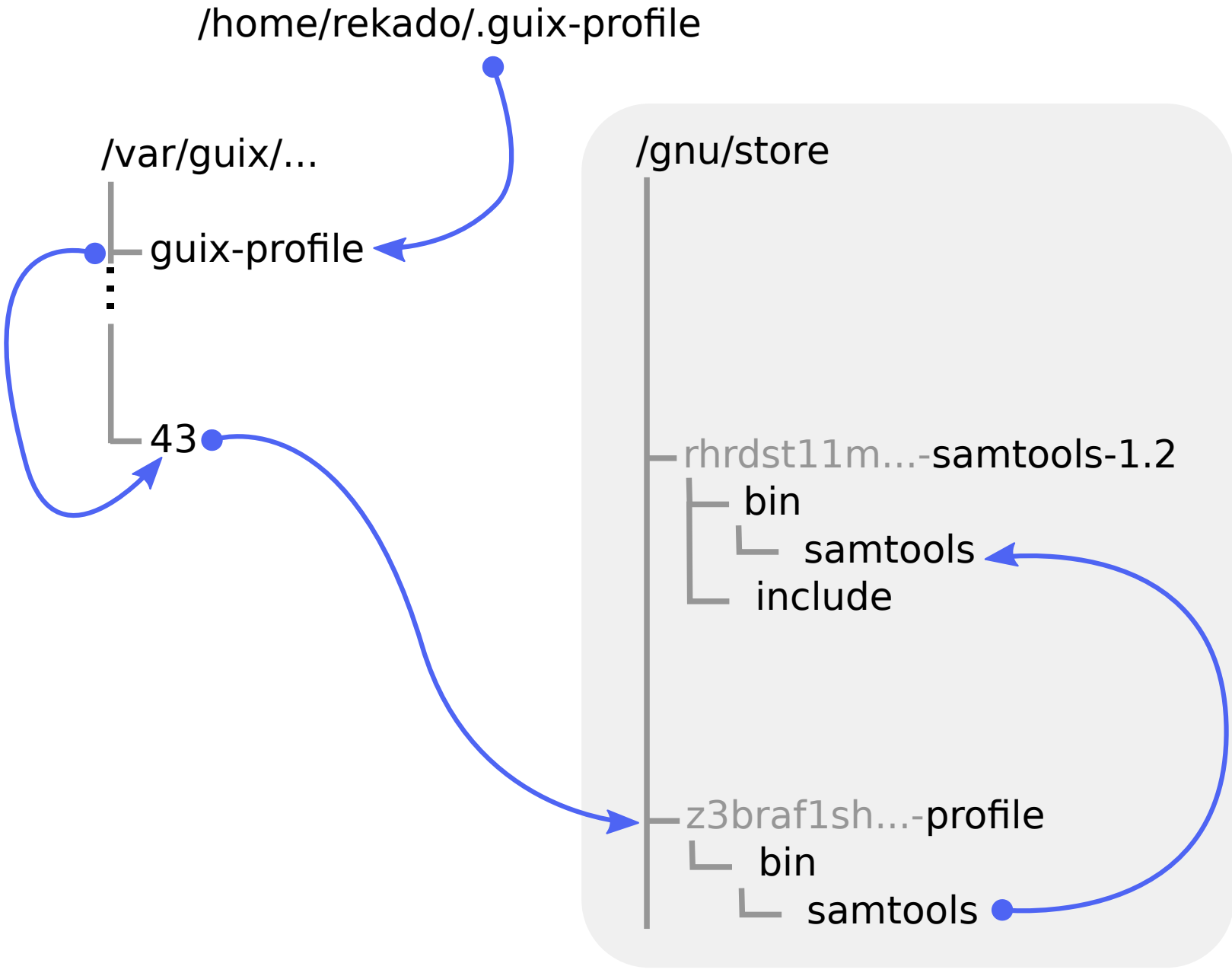
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