GNU Guix and Open science, a crush?

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Université Paris Cité

2013: *Recurrent mutations at codon 625 of the splicing factor SF3B1 in uveal melanoma*
(Nature Genetics) (link)

$\longrightarrow$ Conclusion A

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Conclusion A $\neq$ Conclusion B $\neq$ Conclusion C

Ah, maybe it's an unique case?

Replication and reproducibility crisis

More than 70% of researchers have tried and **failed to reproduce** another scientist's experiments, and more than half have failed to reproduce their own experiments.

1,500 scientists lift the lid on reproducibility (Nature, 2016) (link)

Many causes... one solution?

Open Science helps

$$\left(\begin{array}{lcl} \text{reproducibility} & = & \text{verification} \\ \text{replicability} & = & \text{validation} \end{array} \right)$$

security and "open science" are two sides of the same coin

1905: *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen*
by A. Einstein

- Only one author, verbal reasoning
- Motivated students are able to check by themselves that all the computations are correct

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by Z. Zin & al.

- 15 authors, references to software
- "[...] we scale language models from 8 million parameters up to ***15 billion* parameters**."
- Code and data seems available... but ~~impossible~~^W hard to check that all is correct

is 15 billion parameters declarative and minimalist computing?

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Among several questions, scientific research is evolving,

what does it mean *scientific research* now?

is 15 billion parameters declarative and minimalist computing?

Open Science

Science = Transparent and Collective
Scientific result = Experiment + Numerical processing

Science in the digital age:

1. Open Article — HAL, BioArxiv
2. Open Data — Data Repositories, Zenodo
3. Open Source — Forges, GitLab, Software Heritage

"Open science", a tautology?

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How to ***glue*** it all?

that's Guix!

"Open science", a tautology?

Digression

"Scientific" knowledge is based on

- being able to read the result
- being able to study all the details and adapt them for your own research
- being able to share with peers
- being able to share your own results adapted from the others

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Wait, it looks like the *free software* definition

free software and scientific research are two sides of the same coin

Challenges about reproducible research in science

From the "scientific method" viewpoint:

controlling the source of variations

$\Rightarrow$ transparent — as with instrument $\approx$ computer

From the "scientific knowledge" viewpoint: (universal?)

- Independent observer must be able to observe the same result.
- The observation must be sustainable (to some extent).

$\Rightarrow$ collective

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In a world where (almost) all is *data*

how to redo later and elsewhere what has been done here and today?

(implicitly using a "computer")

Computational environment

Alice says: *"using this data, you need this C file and GCC@11.2.0 to run my analysis"*

- What is source code?
- What are the tools required for building?
- What are the tools required at run time?
- And recursively for each tool...

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How to capture the answer to these questions?

Usually: package manager (Conda, APT, Brew, ...); Modulefiles; container; etc.

Solution(s)

1. package manager: APT (Debian/Ubuntu), YUM (RedHat), etc.
2. environment manager: Conda, Pip, Modulefiles, etc.
3. container: Docker, Singularity

APT, Yum Hard to have several versions or rollback?

Pip/Conda Transparency?

who knows what's inside PyTorch with `pip install torch`? (link)

Modulefiles How are they maintained? (who uses them on their *laptop*?)

Docker Dockerfile based sur APT, YUM, etc.

```
RUN apt-get update && apt-get install
```

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1. package manager: APT (Debian/Ubuntu), YUM (RedHat), etc.
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Guix = #1 + #2 + #3

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Guix: computational environment manager on *steroids*

a **package manager**	(as APT, Yum, etc.)
transactional and declarative	(rollback, concurrent versions)
which produces shareable ***packs***	(Docker or Singularity container)
which produces **isolated *virtual machines***	(*à la* Ansible or Packer)
used to build a whole Linux distribution	(better than other? :-))
... and also a Scheme library...	(extensibility!)

Guix runs on top of a Linux distribution, or standalone.

Easy to try

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20 minutes. . .

. . . is a quick summary calling for your own experimentation (maybe?)

(this talk is a small *snack*)

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Guix: computational environment manager on *steroids*

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- which produces reproducible packs
- which produces isolated virtual machines
- used to build a whole Linux distribution
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- (rollback, concurrent versions)
- (Docker or Singularity containers)
- (a la Ansible or Packer)
- (better than other?)
- (extensibility)

how Guix is helping me

20 minutes...

...is a quick summary calling for your own experimentation (maybe?)

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Guix runs on top of a Linux distribution, or standalone.

Easy to try

Guix, really yet another package manager?

- Package install/remove without any special privilege
- Declarative management (declarative = configuration file)
- Transactional (= no « *broken* » state)
- Binary *substitutes* (= fetch pre-compiled components)

- Isolated environment *on-the-fly* (`guix shell --container`)
- Factory for *images* (`guix pack -f docker`)

The *profiles* allow to install several versions.

(*profile* ≈ "environment *à la* `virtualenv`")

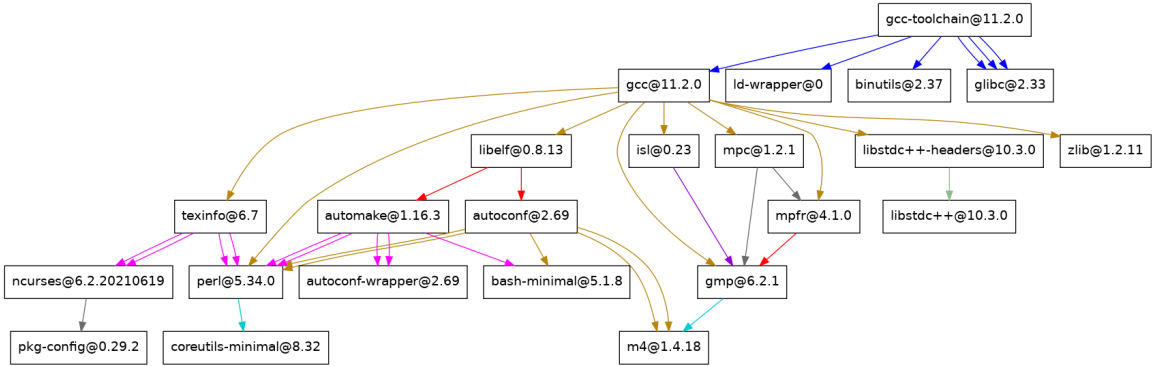
Interesting features, but why is the computational environment controlled (*reproducible*)?

We need to talk about version!

Example: Alice and Blake are collaborating

When Alice says “GCC at version 11.2.0”

`guix graph`



Is it the same “version” of GCC if `mpfr` is replaced by version 4.0?

complete graph: 43 ou 104 ou 125 ou 218 nodes
(depending what we consider as *binary seed* for *bootstrapping*)

What is my version of Guix?

`guix describe` = state

```
$ guix describe
Generation 76 Apr 25 2022 12:44:37 (current)
  guix eb34ff1
    repository URL: https://git.savannah.gnu.org/git/guix.git
    branch: master
    commit: eb34ff16cc9038880e87e1a58a93331fca37ad92

$ guix --version
guix (GNU Guix) eb34ff16cc9038880e87e1a58a93331fca37ad92
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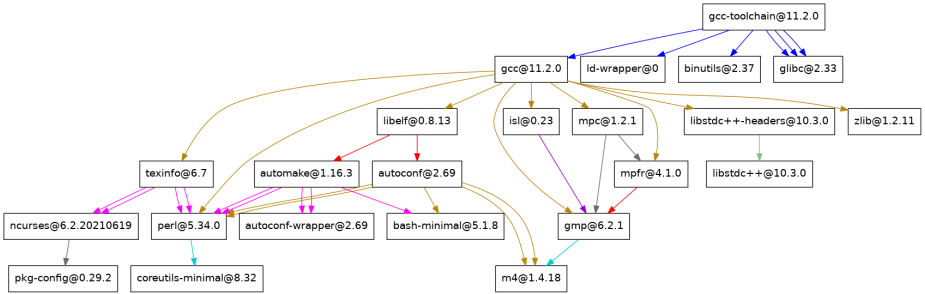
```

one state **pins** the complete collection of packages and Guix itself

A state can refer to several channels (= Git repository), pointing to URL, branches or commits different
A channel contains a list of recipes (code source, how to build the packages, etc.)

State = Directed Acyclic Graph(*DAG*)



Each node specifies a recipe defining:

- code source — and potentially some *ad-hoc* modifications (`patch`)
- build-time tools — compilers, build automation, configuration flags etc.
- dependencies — other packages ($\rightarrow$recursive $\rightsquigarrow$ graph)

Complete graph : Python = 137 nodes, Numpy = 189, Matplotlib = 915, Scipy = 1439 nodes

Alice

describes her environment:

- the list of the tools using the file `manifest.scm`, spawns her environment e.g.,

```
guix shell -m manifest.scm
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guix describe -f channels > state-alice.scm
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collaborate = share one computational environment

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Blake

spawns the same computational environment **from these two files**

```
guix time-machine -C state-alice.scm -- shell -m manifest.scm
```

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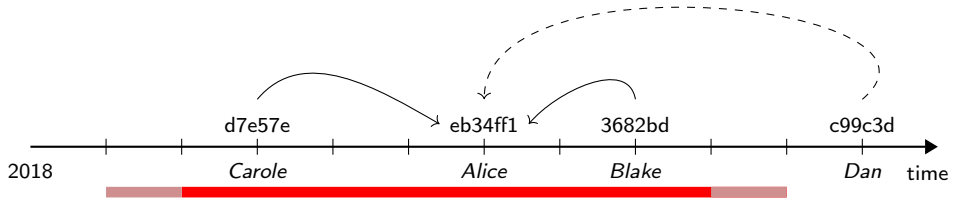
Carole can also reproduce the same environment as Blake (and thus Alice)

Reproducible = jump to different states

`guix time-machine`



Requirements for being reproducible with the passing of time using Guix:

- Preservation of the **all** source code ($\approx$ 75% archived (link) in Software Heritage (link))
- *Backward* compatibility of the Linux kernel
- Compatibility of *hardware* (to some extent)

What is the size of this temporal window where these 3 conditions are satisfied?

To my knowledge, the Guix project is quasi-unique by experimenting since v1.0 in 2019.

Preservation with Software Heritage (= source code long term archive)

`https://www.softwareheritage.org/`

collect and **preserve** software in source code form in the very long term
(not a forge!)

Guix is able:

- save source code from Guix package definition and the Guix package definition itself
- use Software Heritage as fallback if source disappears

Questions:

- How to cite a software? Reference to source code only? Dependencies? Build options?
- **Intrinsic** identifier *(depends only on the object; as checksum)*
  vs **Extrinsic** identifier
  (depends on a register to keep the correspondence between identifier and object; as label version)

Wait, my collaborators do not run Guix

Guix is helping me (2/2)

How to create a container?

Example: Alice wants to share a Docker image

How to capture an environment for sharing? with a container, right?

Container = smoothie :-)

- How to build the container? Dockerfile?
- How the binaries included inside the container are they built?

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```
FROM amd64/debian:stretch
RUN apt-get update && apt-get install git make curl gcc g++ ...
RUN curl -L -O https://...  && ...  && make -j 4 && ...
RUN git clone https://... && ... && make ... /usr/local/lib/libopenblas.a ...
```

(seen for nightly automation; maybe used in production?)

Considering one Dockerfile at time t, how to rebuild the image at time t'?

pack = collection of packages stored in one archive format

What is the aim of a *pack*?

- Alice provides « everything » to Blake,
- Blake does not have Guix but will run the exact same environment.

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What does it mean an archive format?

- `tar` (*tarballs*)
- Docker
- Singularity
- Debian binary package `.deb`
- RPM package `.rpm`

What does it mean « everything »?

Blake needs *transitive closure* (= all the dependencies)

```
$ guix size python-numpy --sort=closure
store item              total    self
python-numpy-1.20.3     301.5    23.6   7.8%
...
python-3.9.9            155.3    63.7  21.1%
openblas-0.3.18         152.8    40.0  13.3%
...
total: 301.5 MiB
```

`guix pack` builds this archive containing « everything »

Building a *pack* for sharing

`guix pack -f docker`

- Alice builds a *pack* using the format Docker

```
guix pack --format=docker -m manifest.scm
```

then shares this Docker container (using some *registry* or else).

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- Blake does not run (yet?) Guix

```
$ docker run -ti project-alice python3
Python 3.9.9 (main, Jan  1 1970, 00:00:01)
[GCC 10.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

and is running the exact same computational environment as Alice.

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```

and is running the exact same computational environment as Alice.

How to rebuild the exact same Docker *pack* using Guix on 2 machines at 2 different moments (link)

Summary, `guix pack` is

Agnostic concerning the « container » format

- `tar` (*tarballs*)
- Docker
- Singularity
- Debian binary package `.deb`
- RPM package `.rpm`

- relocatable binaries
- **without** `Dockerfile`
- using `squashfs`
- without `debian/rule` (experimental)
- without RPM machinery (`patch#61255`)

Flexible to contexts

the **key point** is the **full control** of binaries going inside the container

Summary

Guix: computational environment manager on *steroids*

Guix is helping me

- 3 commands + 2 files for sharing computational environments
  - `guix shell -m manifest.scm`
  - `guix time-machine -C channels.scm -- subcommand`
  - `guix describe -f channels > channels.scm`
- "packing factory" for sharing computational environments on infrastructure without Guix

Guix precisely controls the complete implicit graph of configurations

`manifest.scm` is **reproducible** at the exact same `channels.scm`

Reproducible from one machine to another with the passing of time

https://hpc.guix.info

- Toward practical transparent verifiable and long-term reproducible research using Guix (Nature Scientific Data, 2022)(link)
- Reproductibilité des environnements logiciels avec GNU Guix (mini-tuto 1h JRES, 2022)(link in French)

https://10years.guix.gnu.org/

FOSDEM 2014 (1), 15 (2), 16 (3 4 5 6), 17 (7 8 9 10 11 12 13 14), 18 (15), 19 (16 17 18 19), 20 (20 21 22 23 24 25), 21 (26 27 28 29), 22 (30 31)

Running in production

Grid'5000		828-nodes	(12,000+ cores, 31 clusters)	(France)
GliCID (CCIPL)	Nantes	392-nodes	(7500+ cores)	(France)
PlaFrIM Inria	Bordeaux	120-nodes	(3000+ cores)	(France)
GriCAD	Grenoble	72-nodes	(1000+ cores)	(France)
Max Delbrück Center	Berlin	250-nodes	+ workstations	(Allemagne)
UMC	Utrecht	68-nodes	(1000+ cores)	(Pays-Bas)
UTHSC Pangenome		11-nodes	(264 cores)	(USA)
(yours?)				

more all laptops and desktops

Finalizing

the message you should get back to home

How to redo later and elsewhere what has been done here and today?

Open Science

Traceability and transparency

being able, collectively, to study bug-to-bug

Guix should manage everything about the computational **environment**

```
guix time-machine -C channels.scm -- shell -m manifest.scm
```

if it is specified

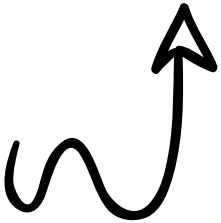
"how to build" `channels.scm`

"what to build" `manifest.scm`

The vision

Software Heritage

The ReScience Journal



Thanks:

- Guix community. You are awesome!
- Ludovic Courtès
- Mathieu Othacehe

Questions?

`guix-science@gnu.org`

`#guix` and `#guix-hpc` on Libera Chat IRC network
dedicated Mattermost (chat) (link)

`https://hpc.guix.info/events/2022/café-guix/`

These slides are archived.
(Software Heritage id swh:1:dir:2494ed717a50f1b9ee33f0c8881017d7cd8e93fd)

Appendix

More about

- Declarative approach
- What a package looks like
- Package transformation
- What the file capturing the state looks like
- Extended environment, isolated

Declarative approach (1/3) `guix shell python python-numpy --export-manifest`

declarative = configuration file

The file `my-tools.scm` could contain this declaration:

```
(specifications->manifest
 (list
  "python"
  "python-numpy"))
```

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

equivalent to

```
guix install python python-numpy
```

Declarative approach (2/3)

Version? We will see later

Language? *Domain-Specific Language* (DSL) based on Scheme (link)

(= « Lisp functional language » (link))

Declarative vs Imperative (links) (and not passive Data vs active Program)

Declarative programming = functional (OCaml) or dataflow (Lustre) or logic (Prolog) programming

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- `(Yes (when (= Lisp parentheses) (baroque)))`
- But **continuum** :
  1. configuration (`manifest`)
  2. package definition (or services)
  3. extension
  4. the core of Guix is Scheme too

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Guix is **flexible** for most needs

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Declarative programming = functional (OCaml) or dataflow (Lustre) or logic (Prolog) programming

Declarative approach: example of transformation (3/3)

Rube Goldberg machine :-) (link)

```
(define python "python")

(specifications->manifest
 (append
  (list python)
  (map (lambda (pkg)
         (string-append python "-" pkg))
       (list
        "matplotlib"
        "numpy"
        "scipy"))))
```

Guix DSL, *variables*, Scheme et chaîne de caractères.

Declarative approach: example of transformation (3/3)

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  "python-matplotlib"
  "python-numpy"
  "python-scipy"))
```

Guix DSL, *variables*, Scheme et chaîne de caractères.

Recipe for defining a package

one node of the graph

```
(define python
  (package
    (name "python")
    (version "3.9.9")
    (source ... )                          ;points to URL source code
    (build-system gnu-build-system)        ;./configure & make
    (arguments ... )                       ; configure flags, etc.
    (inputs (list bzip2 expat gdbm libffi sqlite
                  openssl readline zlib tcl tk))))
```

Note the terminology (`inputs`, `arguments`) as in mathematical function definition

- Each `inputs` is similarly defined (recursion → graph)
- There is no cycle (bzip2 or its `inputs` cannot refer to `python`)

What are the root of the graph? Part of the broad *bootstrapping* (link) problem

Package transformation (1/2)

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package = recipe for configuring, building and installing a software

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The recipe defines:

- code source and potentially some *ad-hoc* modifications (`patch`)
- build-time tools (compilers, build automation, etc., e.g. `gcc`, `cmake`)
- dependencies (= other packages)

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- dependencies (= other packages)

package transformation allows to rewrite them

Package transformation (2/2)

```
guix package --help-transformations
```

```
--with-source       use SOURCE when building the corresponding package
--with-branch       build PACKAGE from the latest commit of BRANCH
--with-commit       build PACKAGE from COMMIT
--with-git-url      build PACKAGE from the repository at URL
--with-patch        add FILE to the list of patches of PACKAGE
--with-latest       use the latest upstream release of PACKAGE
--with-c-toolchain  build PACKAGE and its dependents with TOOLCHAIN
--with-debug-info   build PACKAGE and preserve its debug info
--without-tests     build PACKAGE without running its tests
--with-input        replace dependency PACKAGE by REPLACEMENT
--with-graft        graft REPLACEMENT on packages that refer to PACKAGE
```

also available using manifest file

Example state-alice.scm

guix describe -f channels-sans-intro

```
(list (channel
        (name 'guix)
        (url "https://git.savannah.gnu.org/git/guix.git")
        (branch "master")
        (commit "00ff6f7c399670a76efffb91276dea2633cc130c"))
      (channel
       (name 'guix-cran)
       (url "https://github.com/guix-science/guix-cran")
       (branch "master")
       (commit "ab70c9b745a0d60a40ab1ce08024e1ebca8f61b9"))
      (channel
       (name 'my-team)
       (url "https://my-forge.my-institute.xyz/my-custom-channel")
       (branch "main")
       (commit "ab70c9b745a0d60a40ab1ce08024e1ebca8f61b9")))
```

Temporary *profile* (1/2)

project-tools.scm

```
(specifications->manifest
 (list
  "python"
  "python-matplotlib"
  "python-numpy"
  "python-scipy"))
```

- Alice would like to quickly jump to a productive environment
- Blake prefers IPython as interpreter

Temporary *profile* (2/2)

```
guix shell -m project-tools.scm                                  # Alice
guix shell -m project-tools.scm python-ipython -- ipython3  # Blake
```

Temporary *profile* (2/2)

```
guix shell -m project-tools.scm                                  # Alice
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```

- `--pure` : clear environment variable definitions (from the parent environment)
- `--container` : spawn isolated container (from the rest of the system)

Temporary *profile* (2/2)

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- `--pure` : clear environment variable definitions (from the parent environment)
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```
guix shell -m project-tools.scm python-ipython                # 1.
guix shell -m project-tools.scm python-ipython --pure         # 2.
guix shell -m project-tools.scm python-ipython --container    # 3.
```

Temporary *profile* (2/2)

```
guix shell -m project-tools.scm                                  # Alice
guix shell -m project-tools.scm python-ipython -- ipython3  # Blake
```

- `--pure` : clear environment variable definitions (from the parent environment)
- `--container` : spawn isolated container (from the rest of the system)
- `--development` : include dependencies of the package

```
guix shell -m project-tools.scm python-ipython                # 1.
guix shell -m project-tools.scm python-ipython --pure         # 2.
guix shell -m project-tools.scm python-ipython --container    # 3.
```

Bonus: `guix shell emacs git git:send-email --development guix`