Guix and long term: difficulties and countermeasures How to redo later and overthere what had be done today and here?

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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? at least, *Open Science* helps

( reproductibility = verification replicability = validation **1905**: Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden by A. Einstein Flüssigkeiten suspendierten Teilchen

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

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**2022**: Evolutionary-scale prediction of atomic level protein structure with a language model 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

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Among several questions\*, scientific research is evolving,

what does it mean *scientific research* now?

\* is 15 billion parameters explanatory?

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

# Science at the digital age:

- 1. Open Article
- 2. Open Data
- 3. Open Source

HAL, BioArxiv Data Repositories, Zenodo Forges, GitLab, Software Heritage

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how to glue all that?

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how to **glue** all that?

today's topic considering long-term (3-5 years)

Redo (reproduce or replicate) a result?								
		audit		opaque		depend?		
result	<i>←</i>	paper	+	data	+	analysis		
data analysis	$\leftarrow$	protocol script	+ +	instruments data	+ +	materials environment		
► a	audit is the « tractable » part							

opaque is generally the hard part

		) a result?					
audit opaque depend?							
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×

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			-				

 $data \leftarrow$  protocol + instruments + materials analysis ← script + data + environment

- audit is the « tractable » part
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- how to evacuate depend? from the equations...

... try to turn environment into audit



\*

Redo	(reproduce	or	replicate)	а	result?
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★ our issue

« computer »  $\approx$  instrument and « computation »  $\approx$  measurement computationnal env. experimental setup  $\leftrightarrow$ 

(universal?)

### Challenges about reproducible research in science

### From the « scientific method » viewpoint:

# controlling the source of variations

 $\Rightarrow$  transparent

as with instrument pprox computer

### From the « scientific knowledge » viewpoint:

- Independant 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 today and here?

(implicitely using a « computer »)

# We will speak about...

# The problem of Alice and Blake

- Package manager
- The Guix's way

# 2 About long-term

- Source code archival: Software Heritage
- Guix in the picture

# 3 Work in progress

(some examples from C programming language but all apply equally to any other computational stack)

Questions (1/2)

Package manager

About long-term

Work in progress

Bessel function  $J_0$  using C programming language

```
#include <stdio.h>
#include <math.h>
```

```
int main(){
    printf("%E\n", j0f(0x1.33d152p+1f));
}
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Package manager

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Alice sees: 5.643440E-08 Blake sees: 5.963430E-08

Determine if the difference is significant or not is let to experts, scientific field by scientific field

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Why? In spite of everything being available (open)

Determine if the difference is significant or not is let to experts, scientific field by scientific field

Package manager

Questions (2/2)

About long-term

Work in progress

Alice and Blake both run  $\ll$  GCC at version 11.2.0  $\gg$ 

Package manager

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About long-term

Work in progress

## Alice and Blake both run $\ll$ GCC at version 11.2.0 $\gg$

still different\*

alice@laptop\$ 5.643440E-08 blake@desktop\$ 5.963430E-08

\*Not an issue with floating-point computations

Package manager

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About long-term

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## Alice and Blake both run « GCC at version 11.2.0 »

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alice@laptop\$	gcc bessel.c		&& ./a.out	
	5.643440E-08			
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(due to *constant folding*\*\*)

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\*\* C language is an example, other source but similar issues with Python, R, Perl, etc.

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Alice and Blake are running two different computationnal environments

### More than version number is required

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# Questions about a computational environment

- What is the code source?
- What are the tools required for building?
- What are the tools required for running?
- ► And recursively for each tool...

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How to capture the answer of these questions?

Usually: package manager (Conda, APT, Brew, ...); Modulefiles; container; etc.  $\Rightarrow$  not enough!

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toward a solution: Guix

About long-term

Package manager

# When Alice says « GCC at version 11.2.0 $\, {\rm >}\,$

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*)

Work in progress

What does reproducing a computational environment mean?

Alice says "GCC at version 11.2.0"

All the tools (node of the graph) must be captured!

#### Remember

Package manager

(due to constant folding)

The	problem	of	Alice	and	Blake
	0000000	000			

About long-term

Work in progress

The Guix's way

# 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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The	problem	of	Alice	and	Blake
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About long-term

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guix (GNU Guix) eb34ff16cc9038880e87e1a58a93331fca37ad92

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.)

About long-term

Work in progress

#### The Guix's way

# 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 (→recursive → graph)
- Complete graph : Python = 137 nodes, Numpy = 189, Matplotlib = 915, Scipy = 1439 nodes

The	problem	of	Alice	and	Blake
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The Guix's way

# Recipe for defining a package

About long-term

Work in progress

### one node of the graph

Each inputs is similarly defined

(recursion  $\rightarrow$ graph)

► There is no cycle

(bzip2 or its inputs cannot refer to python)

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

The Guix's way

About long-term

Work in progress

# Package manager = graph manager

How to capture this information?

- What is the source code ?
- What are the tools required for building?
- What are the tools required for running?
- How is each tool produced?

source

```
inputs, propagated-, native-inputs
```

build-system, arguments
The	problem	of	Alice	and	Blake
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About long-term

Work in progress

# Package manager = graph manager

How to capture this information?

```
What is the source code ?
                                                                          source
  What are the tools required for building?
                                        inputs, propagated-, native-inputs
  ▶ What are the tools required for running?
  How is each tool produced?
                                                         build-system, arguments
                                        ;definition of the node python
 (define python
   (package
      (name "python")
      (version "3.9.9")
      (source ... )
                                             ; points to URI source code
                                             ;./configure & make
      (build-system gnu-build-system)
      (arguments ... )
                                             ; configure flags, etc.
                                             ;other nodes -> graph (DAG)
      inputs (list bzip2
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                          Guix and long term: difficulties and countermeasures
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```

The Guix's way

About long-term

Work in progress

## Revision = one specific graph

« GCC at version 11.2.0 » = one pinned graph

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```

this revision eb34ff1 captures the complete graph

- Alice says « I used Guix at revision eb34ff1 »
- Blake knows all for reproducing the same environment

## Collaboration in action

About long-term

Work in progress

#### Guix is helping

### Alice

describes her environment:

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

guix shell -m manifest.scm

## Collaboration in action

About long-term

Work in progress

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the revision (Guix itself and potentially all the other channels)

guix describe -f channels > state-alice.scm

The Guix's way

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collaborate = share one computational environment

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guix describe -f channels > state-alice.scm

then shares these two files: state-alice.scm and manifest.scm

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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



Requirements for being reproductible 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*
- (No time-bomb!)

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

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

(to some extent)

Preservation of what? and why?

Work in progress

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

Traceability and transparency

being collectively able to study bug-to-bug

Guix should manage everything

about the environment

guix time-machine -C state.scm -- cmd -m list-software.scm

if it is specified

 $\ll$  how to build  $\gg$ 

« what to build »

channels.scm (state)

manifest.scm (software list)

Preservation of what? and why?

Work in progress

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channels.scm (state)

manifest.scm (software list)

What is required in addition to these 2 files?

Preservation of what? and why?

# Preservation of what? (1/3)

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

★ each channel used by channels.scm (= Git repository defining packages)
 ★ code source used by manifest.scm (= URI pointing to upstream)

```
(define python
(package
  (name "python")
  (version "3.9.9")
  (source ...)
  (build-system gnu-build-system)
  (arguments ...)
  (inputs (list ...)))); package definition
```

Preservation of what? and why?

# Preservation of what? (2/3)

## example of source

#### Preservation of what? and why?

## About long-term

Work in progress

# Préservation de quoi ? (3/3)

<ul> <li>Git repository</li> </ul>	(channel)
▶ source	
archive tarballs (compressed)	url-fetch
Git repository	git-fetch
Subversion repository	svn-fetch
Mercurial repository	hg-fetch
<ul> <li>CVS repository</li> </ul>	cvs-fetch

#### Preservation of what? and why?

## About long-term

Work in progress

# Préservation de quoi ? (3/3)

Git repository	(channel)
▶ source	
archive tarballs (compressed)	url-fetch
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Mercurial repository	hg-fetch
CVS repository	cvs-fetch

\$ guix	repl	 sources.scm	sort	uniq	- C	L	sort	-nr	
		13432	url-fetch						
		6691	git-fetch						
		391	svn-fetch						
		43	other						
		31	ng-fetch						
		3	cvs-fetch						

Preservation of what? and why?

## About long-term

# Why preserving?

### Because online services sometimes stop

- ► Google Code (link) early 2016
- Alioth (Debian) in 2018 replaced by Salsa
- ► Gna! in 2017 after 13 years
- ► Gitourious in 2015 (the second most popular service for hosting Git repository in 2011)

etc.

Preservation of what? and why?

### About long-term

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etc.

gforge.inria.fr for example Guix issue #42162 (link) Believe it or not, gforge.inria.fr was finally phased out on Sept. 30th. And believe it or not, despite all the work and all the chat :-), we lost the source tarball of Scotch 6.1.1 for a short period of time (I found a copy and uploaded it to berlin a couple of hours ago).

The	probl	em	of	Alice	and	Blake	
		000	000				

Source code archival: Software Heritage

# How to preserve?

About long-term

Work in progress

## $\mathsf{Forge} \neq \mathsf{Archive}$

collaborative software platform for developing

L'objectif d'une forge est de permettre à plusieurs développeurs de **participer ensemble au développement** d'un ou plusieurs logiciels, le plus souvent à travers le réseau Internet.

https://fr.wikipedia.org/wiki/Forge\_(informatique)

## (no English wikipedia entry)

L'archivage est un ensemble d'actions qui a pour but de garantir l'accessibilité sur le long terme d'informations (dossiers, documents, données) que l'on doit ou souhaite conserver pour des raisons juridiques

https://fr.wikipedia.org/wiki/Archivage

Software Heritage « are building the universal software archive » (link)

Source code archival: Software Heritage

## Online service sometimes stop...

Why would it be different for Software Heritage?

No guarantee but...

Software Heritage is an open, non-profit initiative unveiled in 2016 by Inria. It is supported by a broad panel of institutional and industry partners, in collaboration with UNESCO.

The long term goal is to collect all publicly available software in source code form together with its development history, replicate it massively to ensure its preservation, and share it with everyone who needs it.

- Strong support by national and international institutes
- ▶ With the mission to specifically archive all the open source code

(SWH demo?)

About long-term

Work in progress

Guix in the picture

## Preservation with Software Heritage

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 archive as fallback if upstream source disappears

Questions:

- ► How to cite a software? Reference to source code only? Dependencies? Build options?
- Intrinsic identifier
   vs Extrinsic identifier
   (depends only on the object; as checksum)

(depends on a register to keep the correspondence between identifier and object; as label version)

Guix in the picture

About long-term

Work in progress

# Guix and Software Heritage (SWH): status

Guix is able to:	
► save	(automatically) source code to SWH
find back	(automatically) source code from SWH

#### But not for all the type of source!

- Current tooling for Guix ecosystem:
  - Git repository
  - archive tarballs (compressed)
- ... and all the rest is still missing

git-fetch url-fetch

About long-term

Work in progress

#### Guix in the picture

## Some stats : preservation of Guix



### https://ngyro.com/pog-reports/latest/

Saved in Software Heritage:

- ▶ Git = 98.3%
- $\blacktriangleright$  tarballs  $\approx$  70%

(need some love for resuming :-))

## As an practitioner

Save the source code of the package

guix lint -c archival some-package

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Manually save the Git repository of third-party channels (the complete recipe = graph)

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Find the source of one package (if "missing") guix help ... bah that's automatic :-) If all is working as expected, this does all the job, guix time-machine -C channels.scm -- shell -m manifest.scm

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Guix tries, in that order,

- is it available in the substitute servers?
- is it available upstream
- ▶ is it in Software Heritage?

(defined by source)?

# Reproducible researcher point of view

Alice implements a software where the source code is at:

https://gitlab.inria.fr/projet/un-outil.git

and package it using this channel:

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- Alice saves in Software Heritage these both Git repositories
- Alice publishes along to the paper the two file channels.scm and manifest.scm

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and package it using this channel:

https://gitlab.inria.fr/projet/un-canal.git

- Alice saves in Software Heritage these both Git repositories
- Alice publishes along to the paper the two file channels.scm and manifest.scm
- Blake is able to redeploy the same computational environment as Alice ...although the inria.fr server machine are down!

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

# Fallback in action

```
$ guix time-machine -C channels.scm -- shell -m manifest.scm
Updating channel 'guix' from Git repository at 'https://git.savannah.gnu.org/gi
Updating channel 'example' from Git repository at 'https://whatever-here.org/dc
SWH: found revision 67c9f2143aa6f545419ae913b4ae02af4cd3effc with directory at
SWH vault: requested bundle cooking, waiting for completion...
swh:1:rev:67c9f2143aa6f545419ae913b4ae02af4cd3effc.git/
[...]
fatal: could not read Username for 'https://github.com': No such device or add
Trying content-addressed mirror at berlin.guix.gnu.org...
Trying to download from Software Heritage ...
SWH: found revision eleefd033b8a2c4c81babc6fde08ebb116c6abb8 with directory at
[...]
```

https://simon.tournier.info/posts/2021-10-25-software-heritage.html

# Cool, but...

How to identify / reference my code?

intrinsic vs extrinsic identifier (link)

tag (v1.2.3) vs hash (20303c0), then which hash? etc.

- How to be sure that the complete graph is saved and preserved?
- How to deal if one node is failing to be rebuild?
- What about *binary bootstrap* (the roots of the graph)?

etc.

Links:

https://lists.gnu.org/archive/html/guix-devel/2023-02/msg00398.html https://lists.gnu.org/archive/html/guix-devel/2023-03/msg00007.html https://lists.gnu.org/archive/html/guix-devel/2023-03/msg00025.html

## Redo the past

Being able to redeploy from now the same computational environment as 3 years ago

It requires:

- Exact same source code
- Rebuild on compatible hardware
- Deterministic rebuild

hard engineering tasks

\$ cp \$(guix build -S hello) hello.tar.gz

\$ gzip -d \$(guix build -S hello) -c | gzip -c > re-hello.tar.gz

\$ guix hash {,re-}hello.tar.gz 086vqwk2wl8zfs47sq2xpjc9k066ilmb8z6dn0q6ymwjzlm196cd 063mn4h9mr4hqipc29dsa0a5bm330n2db8qy6hb5w5qs75mgldpb guix shell disarchive guile-lzma guile

```
$ disarchive disassemble re-hello.tar.gz
        (sha256
        "eb36fa6a391a175e16341ea3d5840563d4551450ba25c16ec490e49a20b17518"))
      (header (mtime 0) (extra-flags 0) (os 3))
      (compressor gnu)
```

\$ guix hash -S nar -H sha256 -f nix-base32 \$(guix build julia-zygote -S)
02bgj6m1j25sm3pa5sgmds706qpxk1qsbm0s2j3rjlrz9xn7glgk

\$ EDITOR=cat guix edit julia-zygote | grep base32 | tail -1
 (base32 "02bgj6m1j25sm3pa5sgmds706qpxk1qsbm0s2j3rjlrz9xn7glgk"))))

\$ guix hash -S git -H sha1 -f hex \$(guix build julia-zygote -S)
3cfdb31b517eec4173584fba2b1aa65daad46e09
\$ guix hash -S nar -H sha256 -f nix-base32 \$(guix build julia-zygote -S)
02bgj6m1j25sm3pa5sgmds706qpxk1qsbm0s2j3rjlrz9xn7glgk

\$ EDITOR=cat guix edit julia-zygote | grep base32 | tail -1
 (base32 "02bgj6m1j25sm3pa5sgmds706qpxk1qsbm0s2j3rjlrz9xn7glgk"))))

\$ guix hash -S git -H sha1 -f hex \$(guix build julia-zygote -S)
3cfdb31b517eec4173584fba2b1aa65daad46e09

Search with swh:1:dir:3cfdb31b517eec4173584fba2b1aa65daad46e09 returns,

https://archive.softwareheritage.org/browse/directory/3cfdb31b517eec...

see API

https://archive.softwareheritage.org/api/1/directory/3cfdb31b517eec...

Work in progress to bridge various intrinsic identifiers?

Discussion about considering NAR hashes:

https://gitlab.softwareheritage.org/swh/meta/-/issues/4538

in this thread:

- explanation of NAR format (link)
- simple Python implementation of NAR format (link)

About long-term

Work in progress

## The vision to *reach*



## **Questions?**

guix-science@gnu.org

dedicated Mattermost (chat) (link)



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