Guix as a tool for reproducible science

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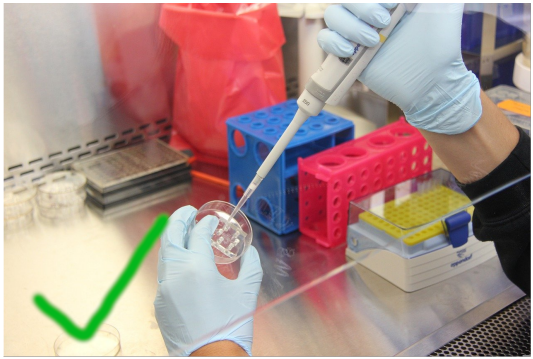
Guix is ...

- a GNU/Linux distribution
- a package manager
- a manager for reproducible containers
- an account configuration manager (tomorrow!)

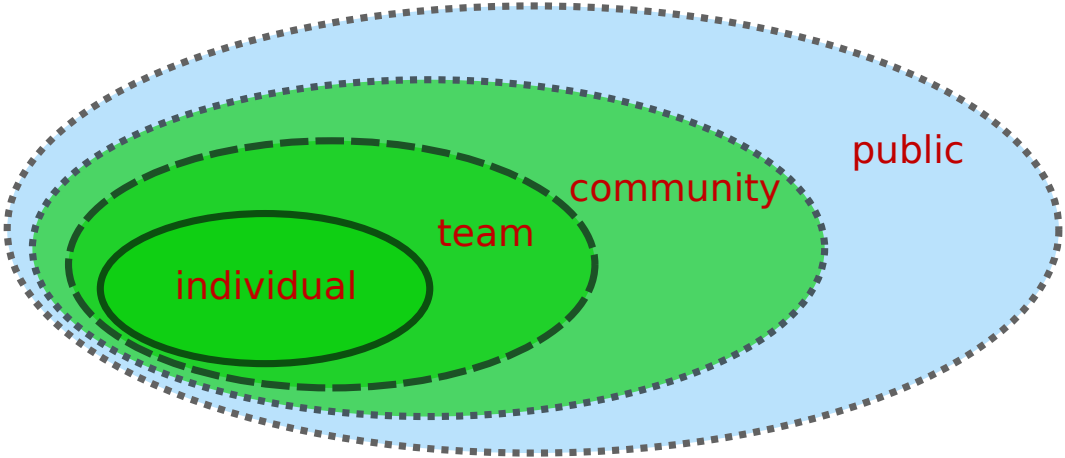
- **a tool for reproducible computation**

Environments matter



Research is not done at `$HOME`, it’s done in a `$LAB`.

Social contexts

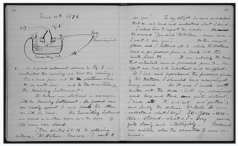


Communication: individual to team

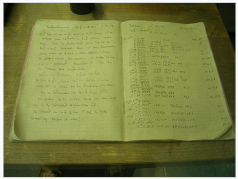
Lab notebook

From Wikipedia, the free encyclopedia

A **laboratory notebook** (*colloq.* **lab notebook** or **lab book**) is a primary record of research. Researchers use a lab notebook to document their hypotheses, experiments and initial analysis or interpretation of these experiments. The notebook serves as an organizational tool, a memory aid, and can also have a role in protecting any intellectual property that comes from the research.[2]



Page from a laboratory notebook of Alexander Graham Bell, 1876.



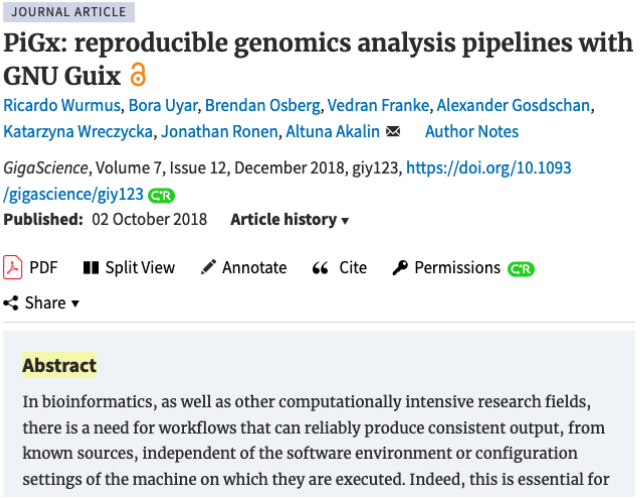
Page from the notebook of Otto Hahn, 1938.

Contents [hide]

Structure [edit]

The guidelines for lab notebooks vary widely between

Communication: team to community



JOURNAL ARTICLE

PiGx: reproducible genomics analysis pipelines with GNU Guix

Ricardo Wurmus, Bora Uyar, Brendan Osberg, Vedran Franke, Alexander Gosdschan, Katarzyna Wreczycka, Jonathan Ronen, Altuna Akalin ✉ Author Notes

GigaScience, Volume 7, Issue 12, December 2018, giy123, https://doi.org/10.1093/gigascience/giy123

Published: 02 October 2018 **Article history** ▾

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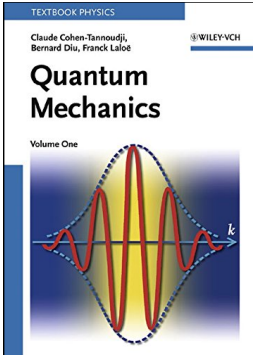
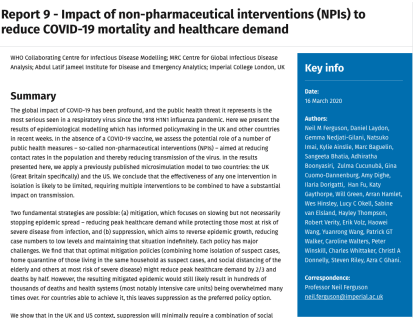
Abstract

In bioinformatics, as well as other computationally intensive research fields, there is a need for workflows that can reliably produce consistent output, from known sources, independent of the software environment or configuration settings of the machine on which they are executed. Indeed, this is essential for

Communication: community to public





Report 9 - Impact of non-pharmaceutical interventions (NPIs) to reduce COVID-19 mortality and healthcare demand

WHO Collaborating Centre for Infectious Disease Modelling; MRC Centre for Global Infectious Disease Analysis; Abdul Latif Jameel Institute for Disease and Emergency Analytics; Imperial College London, UK

Summary

The global impact of COVID-19 has been profound, and the public health threat it represents is the most serious seen in a respiratory virus since the 1918 H1N1 influenza pandemic. Here we present the results of epidemiological modelling which has informed policymaking in the UK and other countries in recent weeks. In the absence of a COVID-19 vaccine, we assess the potential role of a number of public health measures – so-called non-pharmaceutical interventions (NPIs) – aimed at reducing contact rates in the population and thereby reducing transmission of the virus. In the results presented here, we apply a previously published microsimulation model to two countries: the UK (Great Britain specifically) and the US. We conclude that the effectiveness of any one intervention in isolation is likely to be limited, requiring multiple interventions to be combined to have a substantial impact on transmission.

Two fundamental strategies are possible: (a) mitigation, which focusses on slowing but not necessarily stopping epidemic spread – reducing peak healthcare demand while protecting those most at risk of severe disease from infection, and (b) suppression, which aims to reverse epidemic growth, reducing case numbers to low levels and maintaining that situation indefinitely. Each policy has major challenges. We find that that optimal mitigation policies (combining home isolation of suspect cases, home quarantine of those living in the same household as suspect cases, and social distancing of the elderly and others at most risk of severe disease) might reduce peak healthcare demand by 2/3 and deaths by half. However, the resulting mitigated epidemic would still likely result in hundreds of thousands of deaths and health systems (most notably intensive care units) being overwhelmed many times over. For countries able to achieve it, this leaves suppression as the preferred policy option.

We show that in the UK and US context, suppression will minimally require a combination of social

Key info

Date:
16 March 2020

Authors:
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Communicating computer-aided research

- Share data
- Share code (the code you care about)
- Share computational environments (the code you don’t care about)

Computational environments

- Tools enabling research and communication
- Formalized and automated research methods
- Must be shared in a team
- Open Science: must be shared with community and public
- Open Science: must be *verifiable* by community and public

Personal computational environments

- Your `$HOME`
- Not shared with anyone else
- Do what you want

$\Rightarrow$ Guix, Debian, Ubuntu, Arch, ...

Computational environments for teams

- Precisely documented (think lab notebook!)
- Easy to inspect and modify
- Can evolve rapidly

$\Rightarrow$ Guix

Computational environments for communities

- Archived for years to decades (like a journal article)
- Must work identically for verifiability
- May require *some* effort to deply
- Forkable

⇒ Guix, Docker + reproducible image, Guix + Docker

Computational environments for the public

- Simple all-in-one user interface
- Must be maintained for as long as the content is relevant
- Must yield equivalent results at all times for verifiability

$\Rightarrow$ Community environment + UI + support + maintenance

Reproducible environments with Guix

The magic incantation

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

```
guix shell -m manifest.scm -- command argument ...
```

Manifests

Guix' alternative to a `Dockerfile`

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

Where are the version numbers?

- Implicitly defined by Guix
- Updating Guix updates all packages in Guix

Reproducible environments

Keep a record of your Guix snapshot

```
guix describe -f channels > channels.scm
```

Use a recorded snapshot

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

The channel file

```
(list (channel
        (name 'guix)
        (url "https://git.savannah.gnu.org/git/guix.git")
        (branch "master")
        (commit
          "35b176daf1a466f136f0b77c03de78f482a30702")
        (introduction
          (make-channel-introduction
            "9edb3f66fd807b096b48283debdcddccfea34bad"
            (openpgp-fingerprint
              "BBB0 2DDF 2CEA F6A8 0D1D  E643 A2A0 6DF2 A33A 54FA")))))
```

Two files define your environment

- `manifest.scm` defines the list of packages
- `channels.scm` defines the versions

Store both files in your version-controlled project directory!

Three types of environment

Extended $HOME environment

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

- Your $HOME environment plus the packages from the manifest
- Not transferable, not reproducible
- Good for testing software, using conflicting packages

Clean environment

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

- Resets all environment variables ($PATH etc.)
- Unrestricted access to local files and network
- Good for isolating software but not data

Containerized environment

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

Containers with privileges

Network access

```
guix shell --container --network -m manifest.scm
```

- Grants unrestricted network access
- No restriction possible

Local file access

```
guix shell --container --expose=/etc/ssl/certs -m manifest.scm
```

- Grants read-only access to a file/directory

```
guix shell --container --share=$HOME/data -m manifest.scm
```

- Grants read and write access to a file/directory

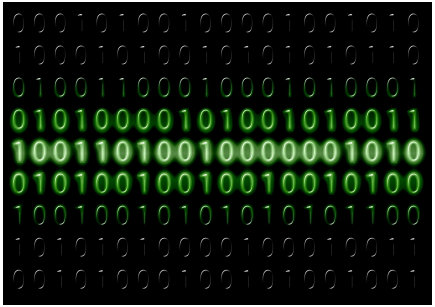
Why Guix rather than Docker?

- Reproducible containers
- Source code for containers
- Source code for all packages in a container
- No huge image files
- Can export to Docker and Singularity

Why Guix rather than Conda?

- Reproducible environments
- Source code for all packages in an environment

The dual nature of software



Summary: reproducible environments

Four commands

- `guix shell`: run in a controlled environment
- `guix describe`: record software versions
- `guix time-machine`: replay software versions
- `guix pull`: update Guix, with all its packages

Two files

- `manifest.scm`: lists your packages
- `channels.scm`: defines versions