Good practices in the lab
Research documentation and electronic notebooks

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Neurocampus Open Science Workshop
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What's expected from Science?

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- Describe and explain **Nature** (human organizations and artificial objects as well)

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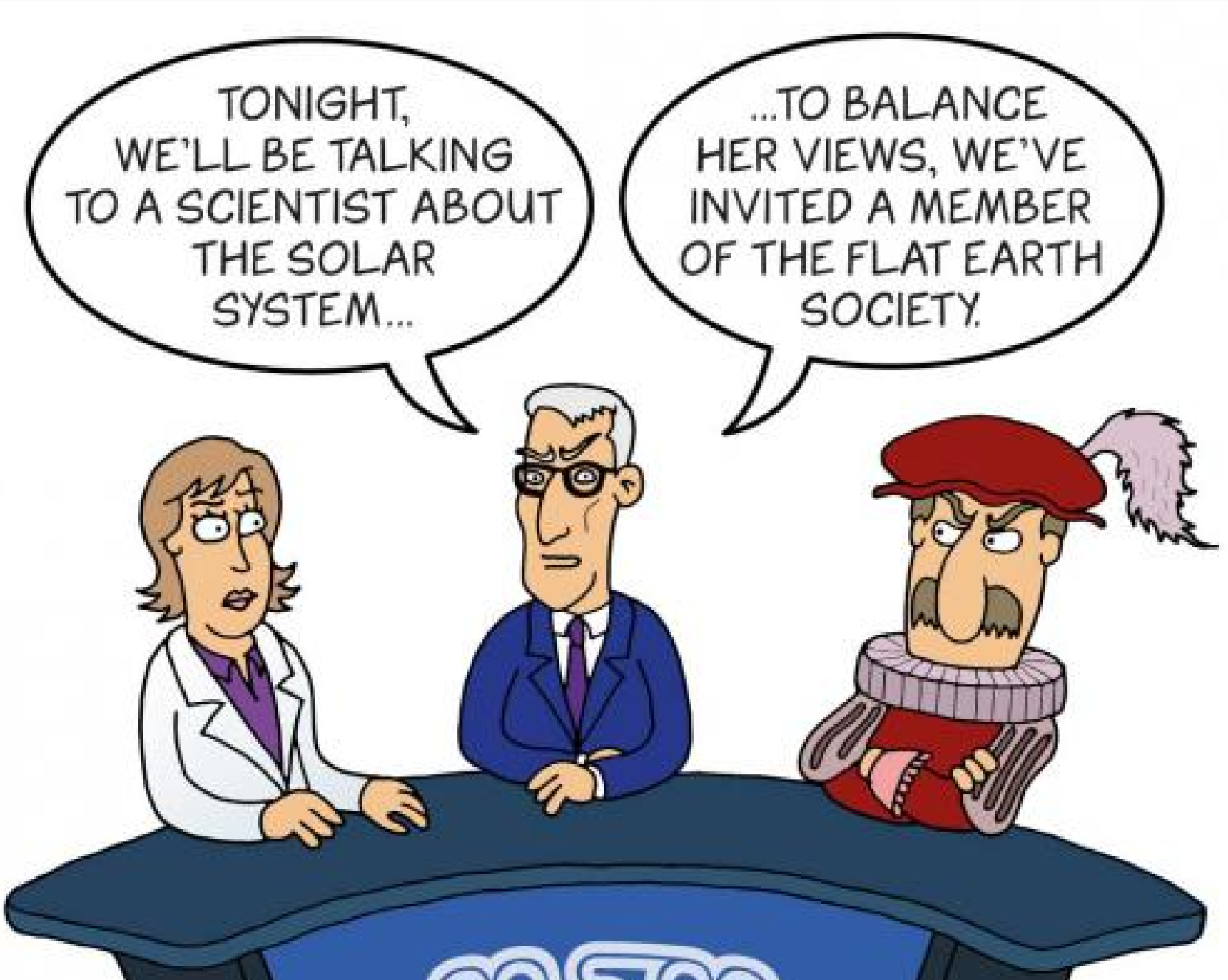
Method

Scientific Consensus



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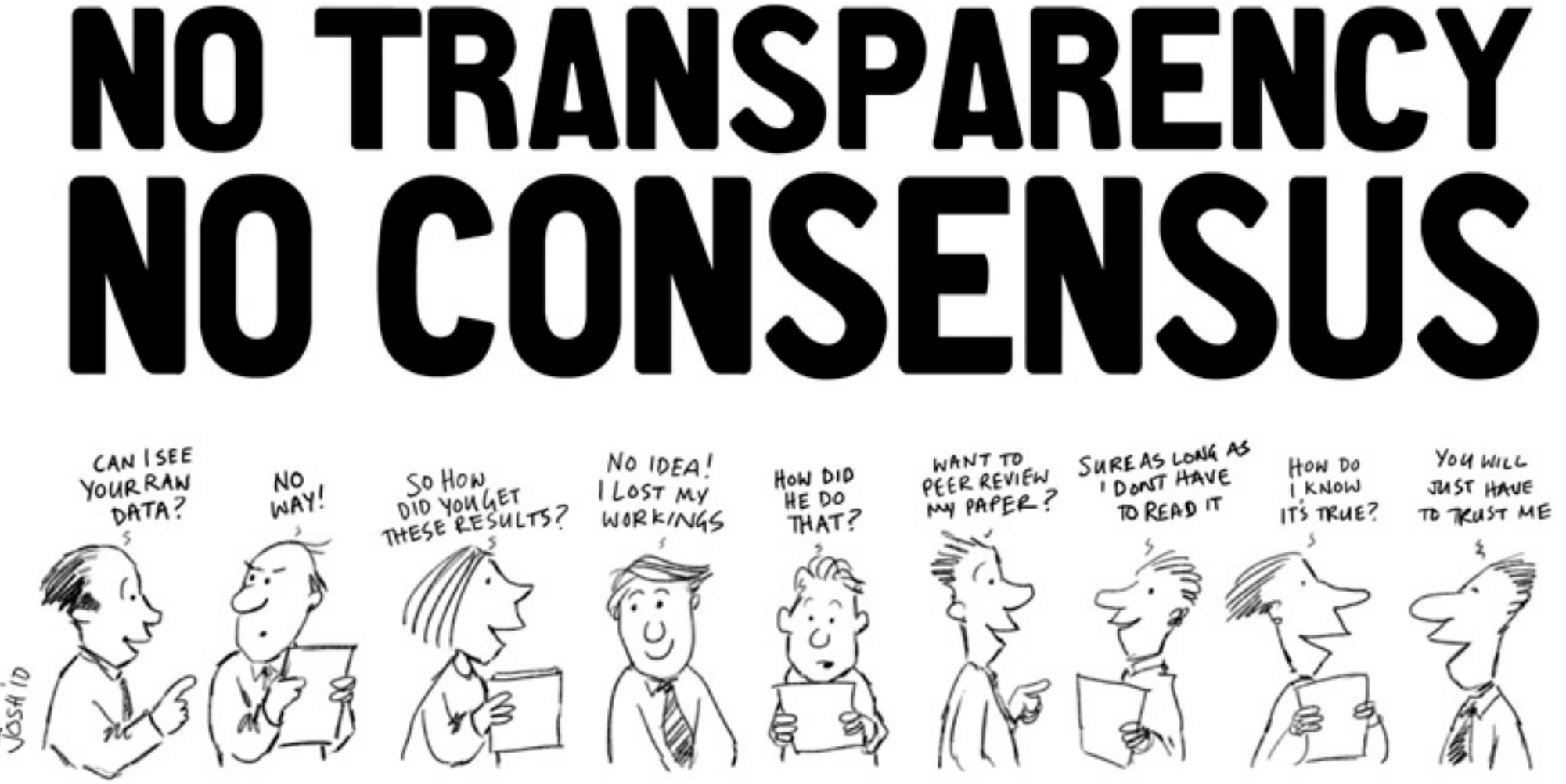

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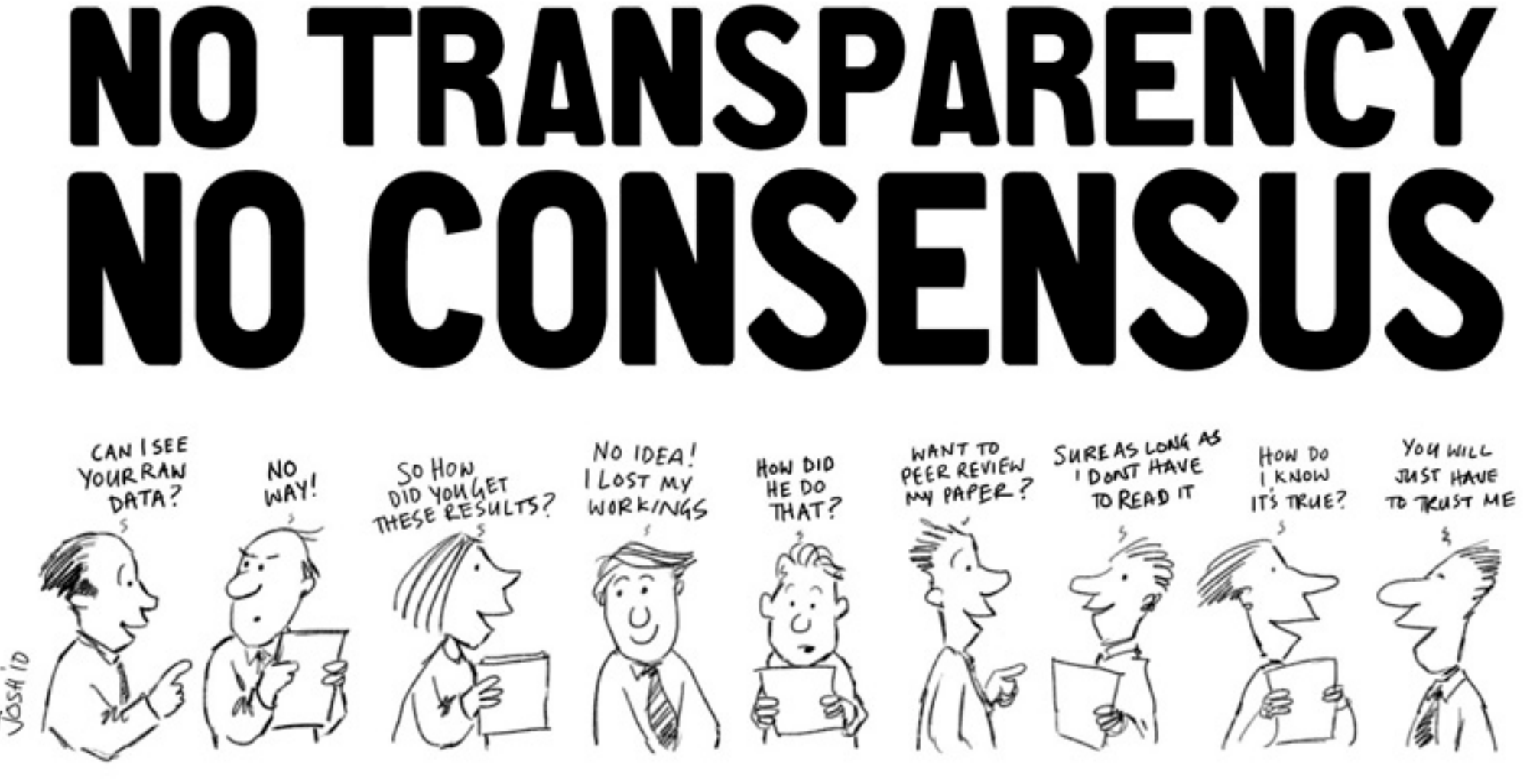

Enlightening the society requires moral/methodological/technical warranties

Merton's four norms of science (1940)

Universalism Scientific validity is independent of the sociopolitical status/personal attributes of its participants (origin, gender, sexuality, religion, etc.)

Communism/communalism All scientists should have common ownership of scientific goods (intellectual property), to promote collective collaboration; secrecy is the opposite of this norm

- We say "Newton's law" to remember that Newton made the original discovery, but not because he has any property of this law

Disinterestedness Scientific institutions act for the benefit of a common scientific enterprise, rather than for the personal gain of individuals

Organized skepticism Scientific claims should be exposed to critical scrutiny (including reproduction) before being accepted

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Merton was not saying *"you should follow these norms"*, but rather

"this is the ~~behavior~~ belief I am observing in the scientific community"

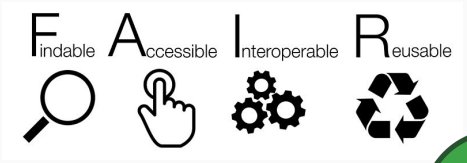
Transparent Research ∼ Open Science ?

Plan National pour la Science Ouverte (BSN ⇝ CoSO)

- CNRS, Inria, INRAE, ...
- Many flavors: *Citizen Science*

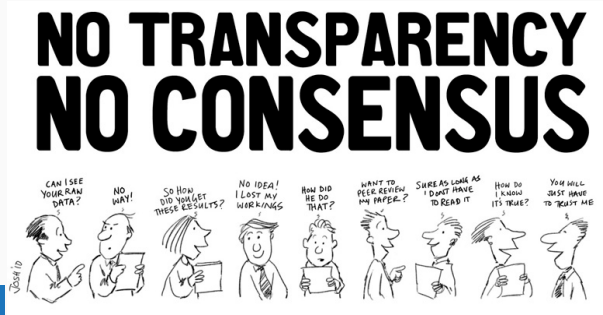
Main pillars:

1. Open access (started before 2000)
2. Open data



CC-BY-SA by default at CNRS!)

3. Open source
   - *Open hardware*
4. **Open methodology** (Reproducible Research)
   - *Open-notebook science*
   - *Open science infrastructures*
5. Open peer review (avoid collusion)
6. Open educational resources



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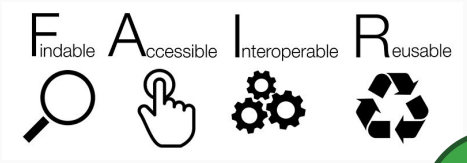

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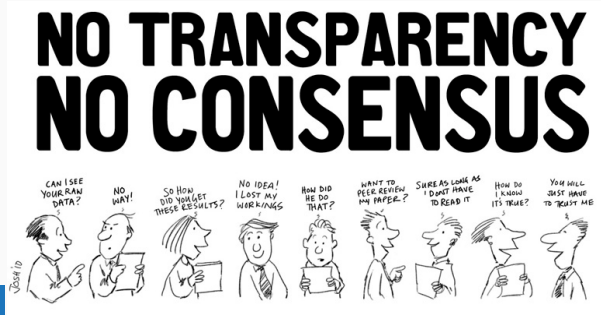

Obviously making code/data available for the reproduction of results from published papers has become the new norm

The scientific Method

Claude Bernard (1865) and Karl Popper (1934)

Observations $\xrightarrow{\text{induction}}$ theory building/proposal

$\xrightarrow{\text{repeated experiments}}$ theory *confirmation*

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(crucial experiment)

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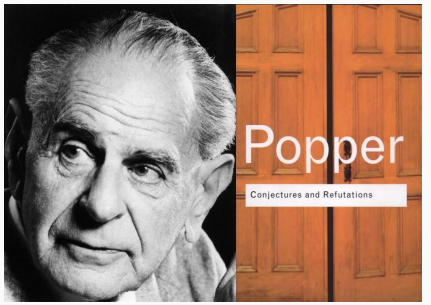

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- Good experiments discriminate good theories from bad ones
- Non-reproducible single occurrences are of no significance to science

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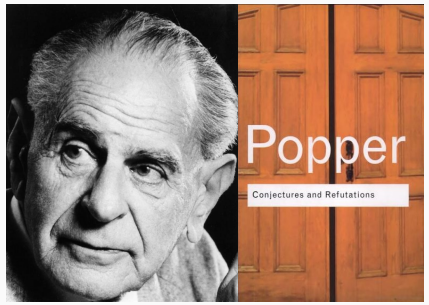

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An ideal rather than the norm

Popper's proposal works well for Physics from the 18th century but is not so simple for many other domains (theory of evolution, astrophysics, particle physics, biology, anthropology)

And in practice ?

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The role of statistics: what are the chances that I observe this by chance (i.e., there is actually no relation but I observe one)?

- Observation $\neq$ experiments (HARKING)
- Selective reporting (p-hacking)

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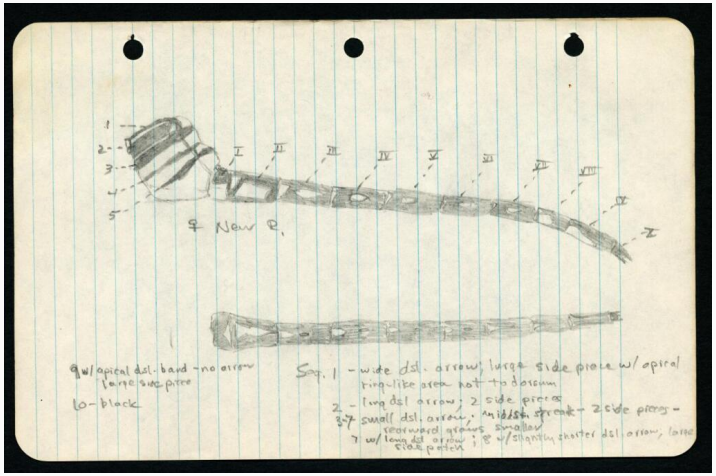
These mistakes require **more than public numbers and raw data**

Notebooks

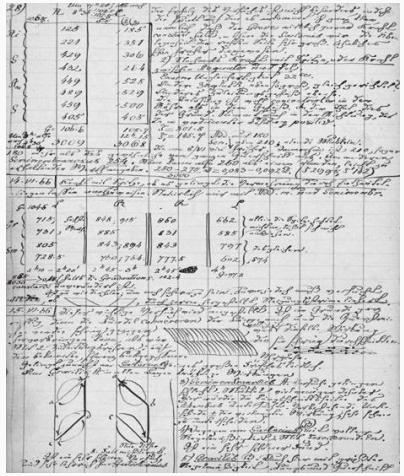
Field and Laboratory notebooks

Social Sciences, Ecology, Biology



Robert Henry Gibbs, Jr.,
ichthyologist (1929 – 1988)

Chemistry, Physics, Biology



Emil Heinrich du Bois-Reymond,
electrophysiology (1818 – 1896)

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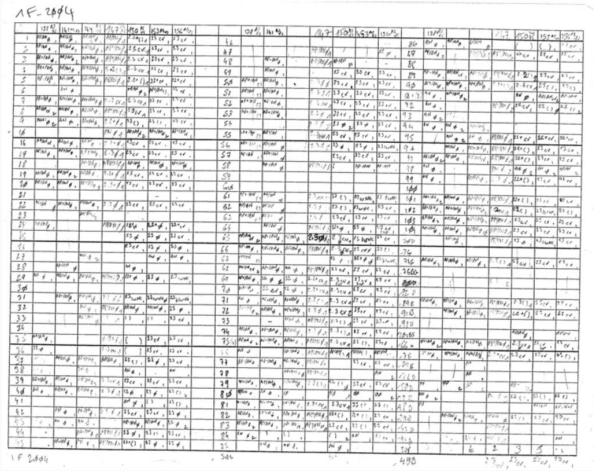

Marie-Claude Quidoz, Centre d'Ecologie Fonctionnelle et Evolutive

Chemistry, Physics, Biology

Contemporary laboratory notebook in Neurology

Essentially no evolution throughout the last century

Pros and Cons

Pros

- Intuitive
- Convenient (lightweight)
- Sketching, equations, thoughts
- *Difficult* to temper

Cons

- Attachments
- Large amount of information
- Indexing and Searching
- No sharing nor backup

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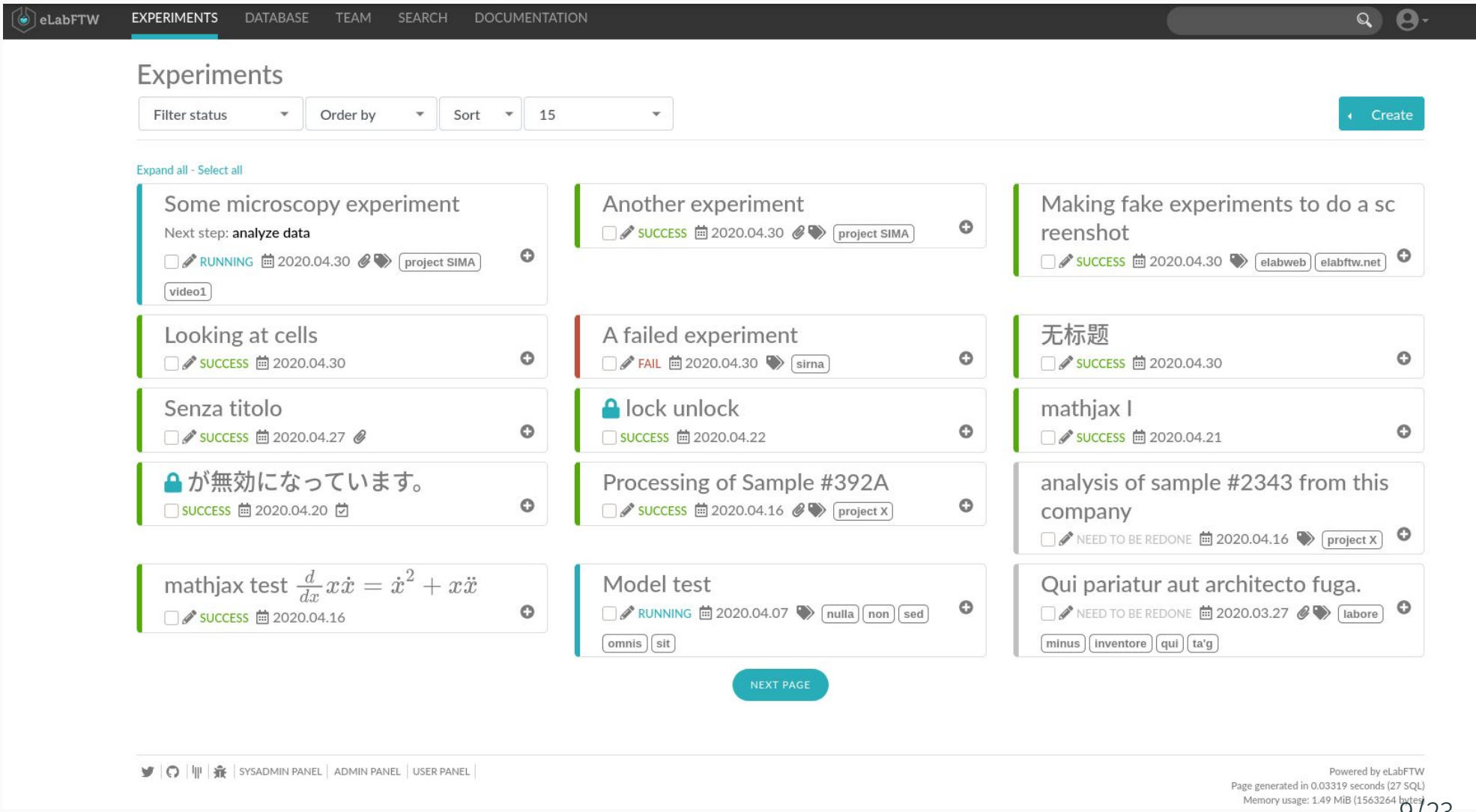
Toward digital notebooks

Electronic Laboratory Notebooks and Laboratory Information Management Systems

- Batch and Sample management
- Instrument integration
- Stock management (e.g., chemical substances)
- Native handling of digital objects

ELN examples 1/2: eLabFTW

eLabFTW: Chemistry @ Lyon (web server w. PHP)



ELN examples 1/2: eLabFTW

eLabFTW: Chemistry @ Lyon (web server w. PHP)

eLabFTW EXPERIMENTS DATABASE TEAM SEARCH DOCUMENTATION

Experiments

Back to listing

2020.04.30 Success Team User

project SIMA video1

Some microscopy experiment

Next step: analyze data

Goal:

Show what an experiment looks like for elabftw.net.

Sample #	Concentration	Absorbance	Density	Something
1	20 µM	0.239	3.4	102
2	30 µM	0.193	4.1	1339

You can have colors too.

And use **bold**, *italics*, underline like you would do in a normal text processing application. Have some mathjax: {x^y}^z is x^{y^z}, and x^{y^z} is x^{y^z}.

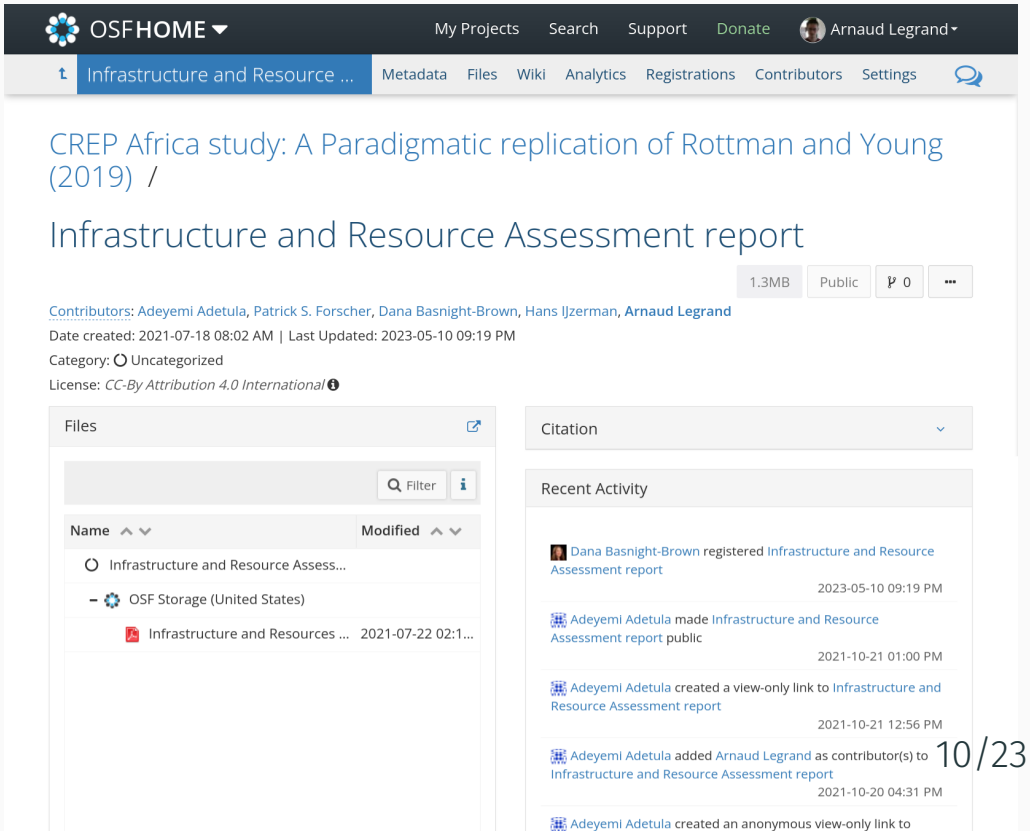
This is a list:

- List item 1
- List item 2
- Now show an image in the text

ELN examples 2/2: OSF.io

A cloud to ease collaboration at the team/lab level

- Shared documents (articles, data, spreadsheets ...)
- Built-in version control
- Integration with Zotero/Mendeley
- Preprints, DMP, Pre-registration, ...
- Social network



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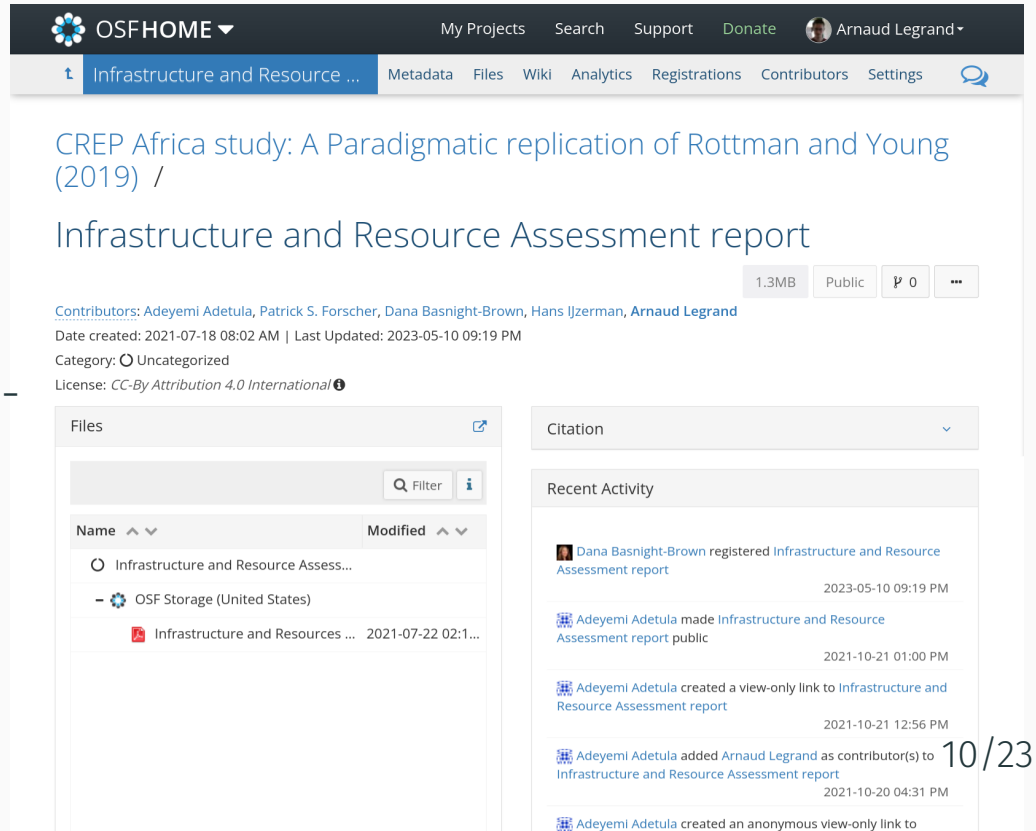
CENTER FOR OPEN SCIENCE

But also

- Dropbox, Google drive storage (privacy? sovereignty?)
- Google/Facebook/ORCID/Institution authentication
- **Locks you in** (huge machinery)
- Nothing done for computations



Damned computers...

How computers broke science –

and what we can do about it

> *Most modern science is so complicated, and most journal articles so brief, it's impossible for the article to include details of many important methods and decisions made by the researcher as he analyzed his data on his computer. How, then, can another researcher judge the reliability of the results, or reproduce the analysis?*

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When moving to the digital world, the rigor is often completely lost.

- Point-and-click procedures are rampant but hinder reproducibility.
- Spreadsheets are generalized and intensively used in biology:
  - `Membrane-Associated Ring Finger (C3HC4) 1`,
    `E3 Ubiquitin Protein Ligase` → `MARCH1` → 2016-03-01 → 1456786800
  - `2310009E13` → 2.31E+19
- And more recently, we had the COVID tracing failure.

Not even mentioning non-mature software and blackbox machine learning procedures

Notes and Documenting

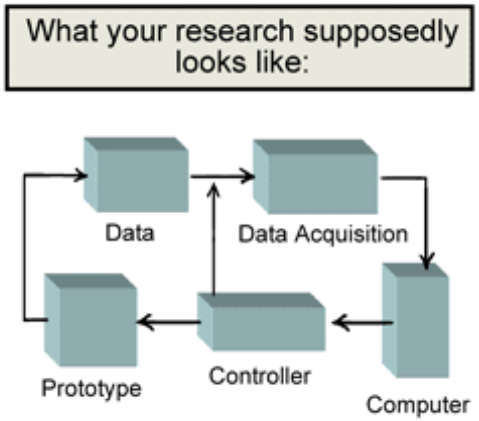

Figure 1. Experimental Diagram

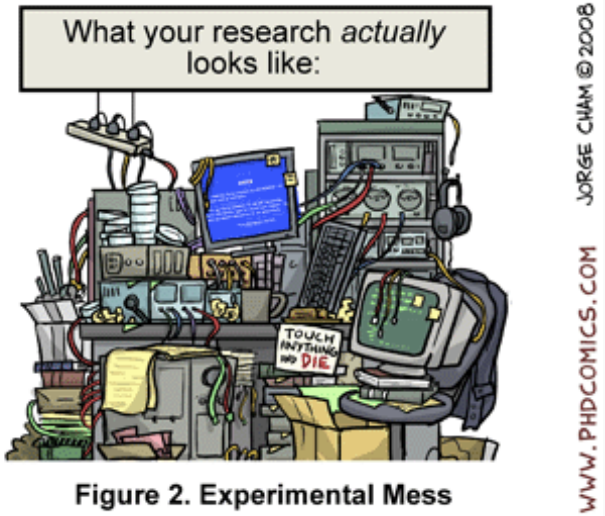

Figure 2. Experimental Mess

Main Challenges for a computational scientist

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Tracking code version

- `my_code` is revision `21b95ecfa0911d6ca87668482b11ab9498edd8f3`

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Handle complex sequences and reuse results (leverage supercomputers)

Tool 1: Computational Notebooks (Litterate Programming)

Un document computationnel

Mon ordinateur m'indique que π vaut *approximativement*

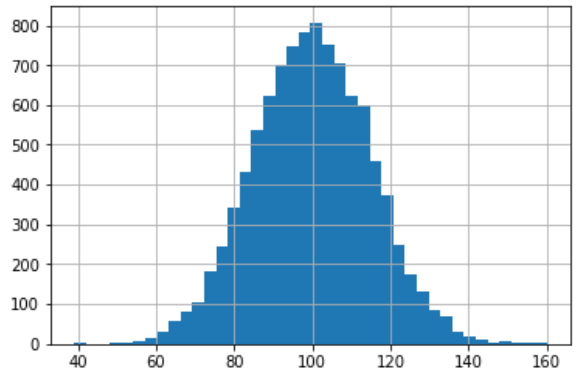
```
3.141592653589793
```

Mais calculé avec la **méthode** des aiguilles de Buffon, on obtiendrait comme **approximation** :

```
import numpy as np
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1)/N)
```

```
3.1437198694098765
```

On peut inclure des formules mathématiques comme $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ et des *dessins qui n'ont rien à voir* avec π (si ce n'est une constante de normalisation... ☺).



Tool 1: Computational Notebooks (Litterate Programming)

Document initial dans son environnement

jupyter example_pi (autosaved)

File Edit View Insert Cell Kernel Widgets Help Hide Code Python 3

Code CellToolbar

Hide Prompts Hide Code Hide Outputs

```
# Un document computationnel
```

Hide Prompts Hide Code Hide Outputs

```
Mon ordinateur m'indique que $\pi$ vaut *approximativement*
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In [1]:

Hide Prompts Hide Code Hide Outputs

```
from math import *
print(pi)
```

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Hide Prompts Hide Code Hide Outputs

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Hide Prompts Hide Code Hide Outputs

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Out[2]: 3.1437198694098765

Hide Prompts Hide Code Hide Outputs

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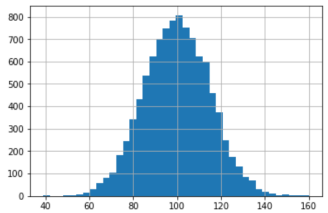
In [3]:

Hide Prompts Hide Code Hide Outputs

```
%matplotlib inline
import matplotlib.pyplot as plt

mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)

plt.hist(x,40)
plt.grid(True)
plt.show()
```



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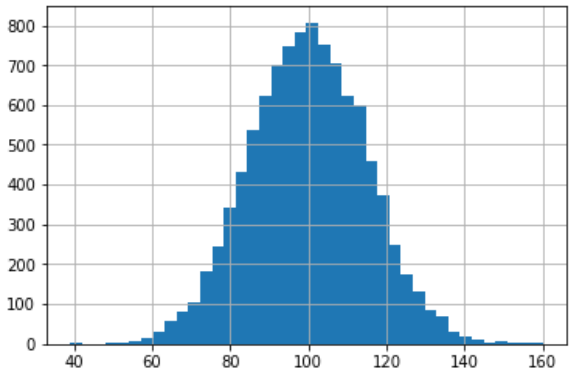

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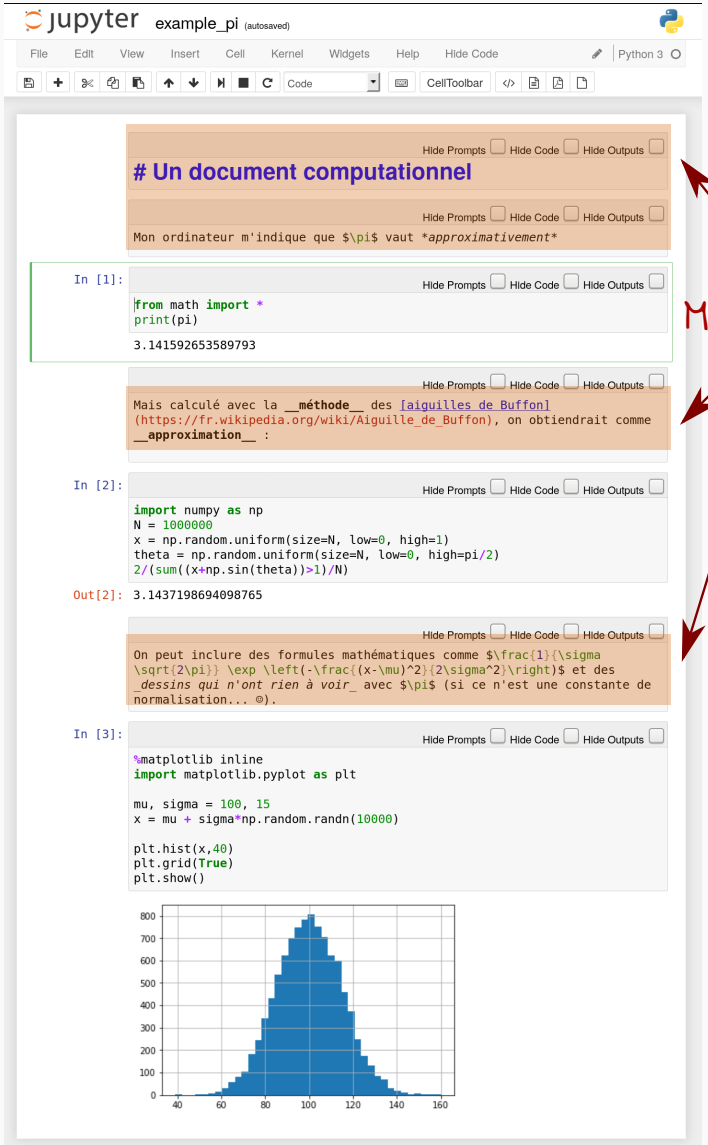

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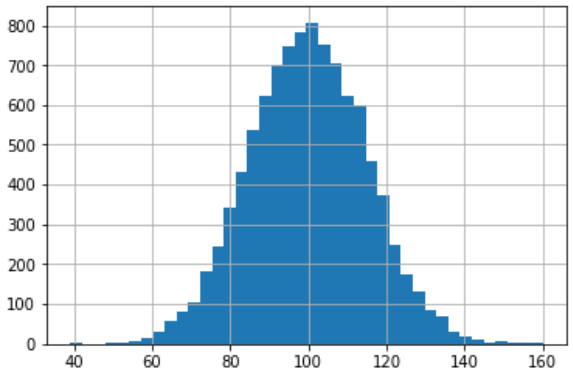
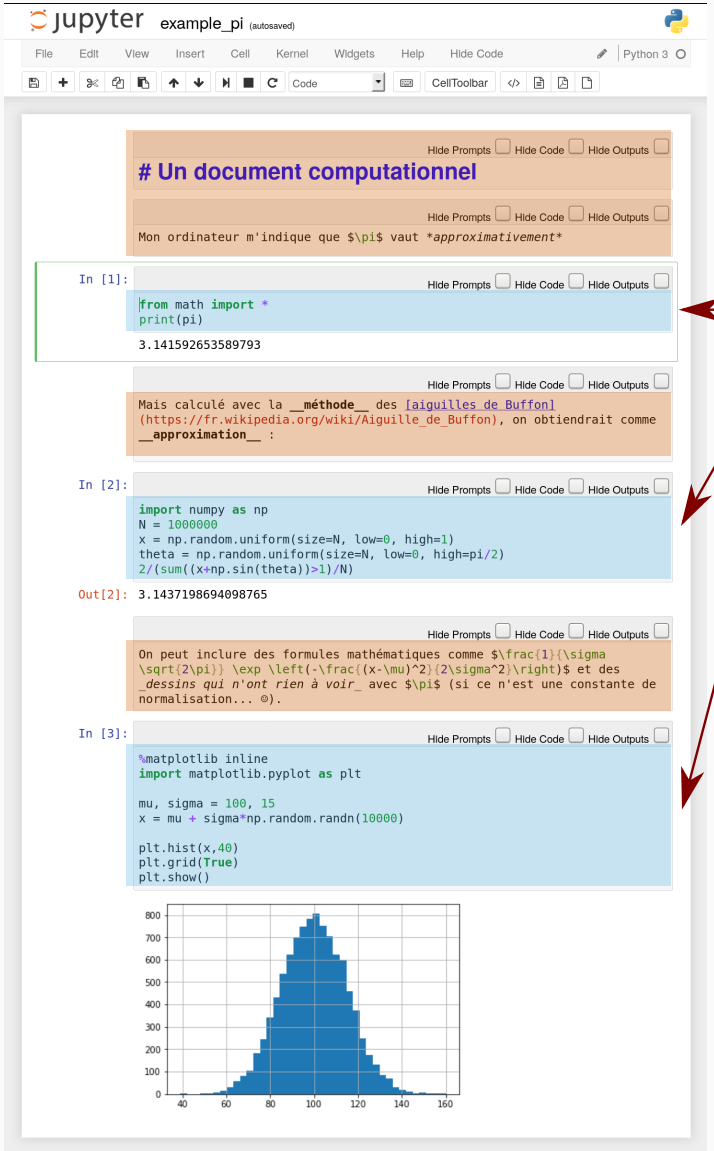


Tool 1: Computational Notebooks (Litterate Programming)

Document initial dans son environnement



Code

Document final

Un document computationnel

Mon ordinateur m'indique que π vaut *approximativement*

```
3.141592653589793
```

Mais calculé avec la **méthode** des aiguilles de Buffon, on obtiendrait comme **approximation** :

```
import numpy as np
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1)/N)
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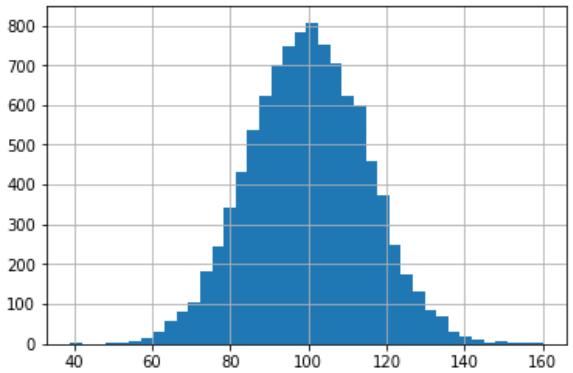

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Document initial dans son environnement

Document final

jupyter example_pi (autosaved)

File Edit View Insert Cell Kernel Widgets Help Hide Code Python 3

Code CellToolbar

Hide Prompts Hide Code Hide Outputs

Un document computationnel

Mon ordinateur m'indique que π vaut *approximativement*

In [1]:

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print(pi)
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In [3]:

```
%matplotlib inline
import matplotlib.pyplot as plt

mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)

plt.hist(x,40)
plt.grid(True)
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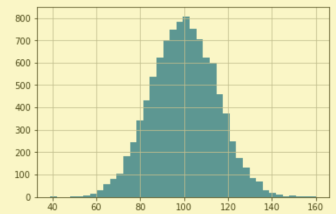

Résultats

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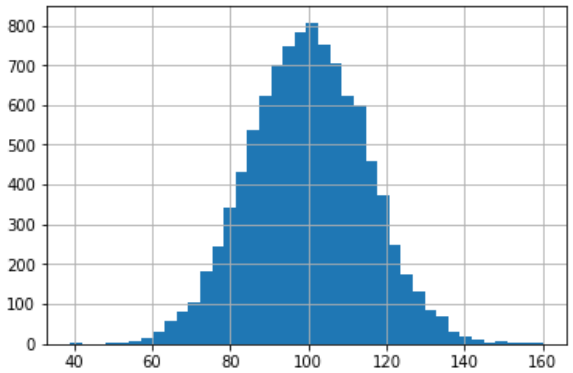

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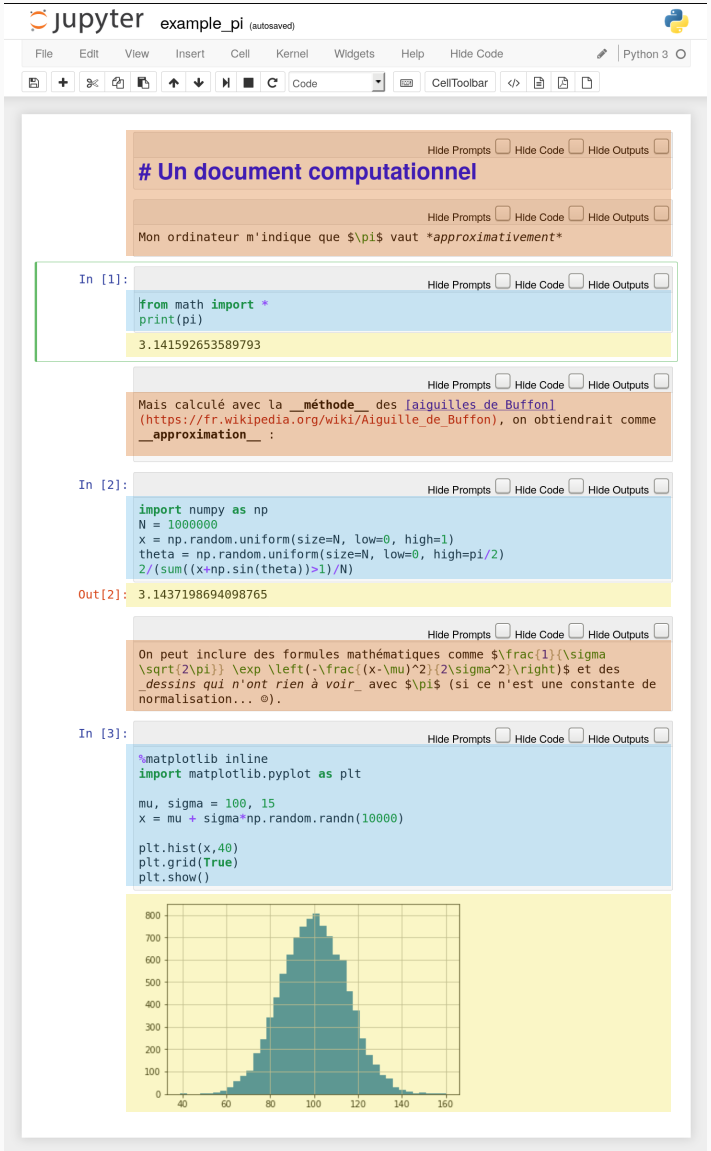

Export

Document final

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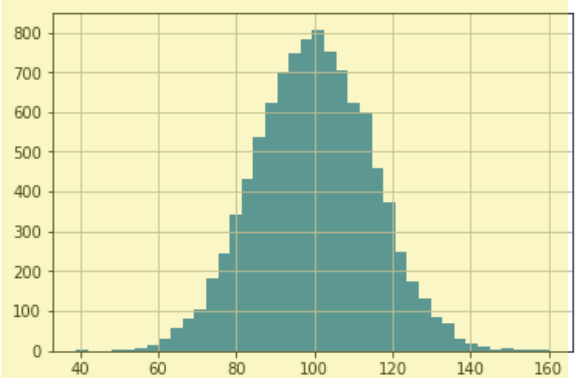

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jupyter example_pi (autosaved)

File Edit View Insert Cell Kernel Widgets Help Hide Code Python 3

Code CellToolbar

Hide Prompts Hide Code Hide Outputs

```
# Un document computationnel
```

Hide Prompts Hide Code Hide Outputs

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Hide Prompts Hide Code Hide Outputs

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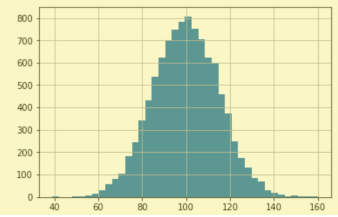

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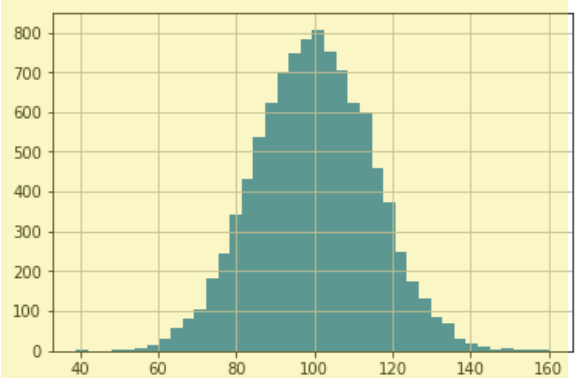

Quick demo of Jupyter, Rstudio, and Org-Mode

(python)

Pros Python/R, friendly, portable (web browser, client/server)

Cons
- Installation, software dependencies (minimal-notebook $\approx$ 440Mb)
- Limited control on typography (unless using *Rube Goldberg* machines like quarto)

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Pros R/Python, friendly, portable, real IDE, Good typography control

Cons
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(emacs-lisp)

Pros R, Python, Perl, Ruby, C, Java, ...
- Pure text, Good typography control, "Lightweight", Programmable editor

Cons
- No default configuration ⇝rough and steep learning curve
- Big machinery: silex/emacs-alpine-ci ≈ 240Mb even though flycheck/emacs-cask ≈ 80Mb

Different reproducibility philosophies

Why and how to use a computational notebook?

The processing steps between raw observations and findings have gotten increasingly numerous and complex

- A reproducible document links raw data with final figures
- What's at stake: verification and reuse by others

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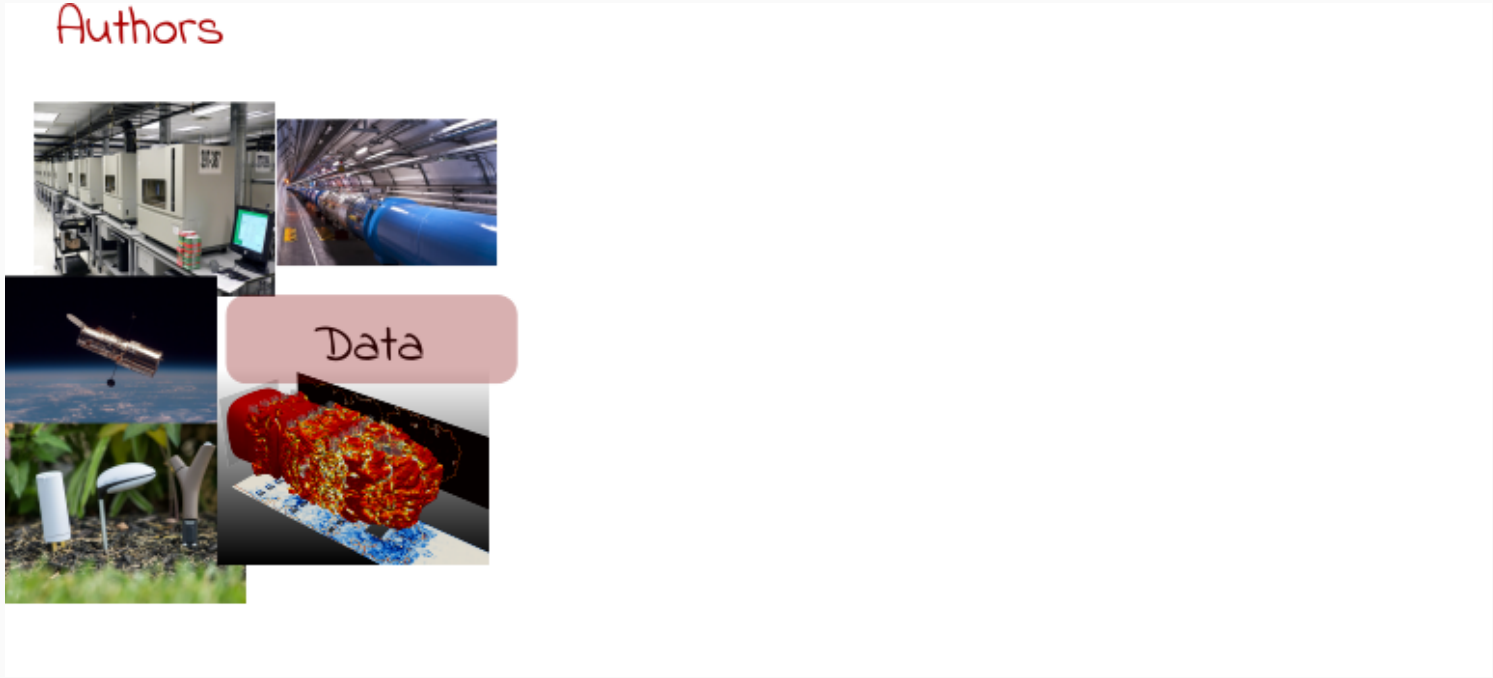

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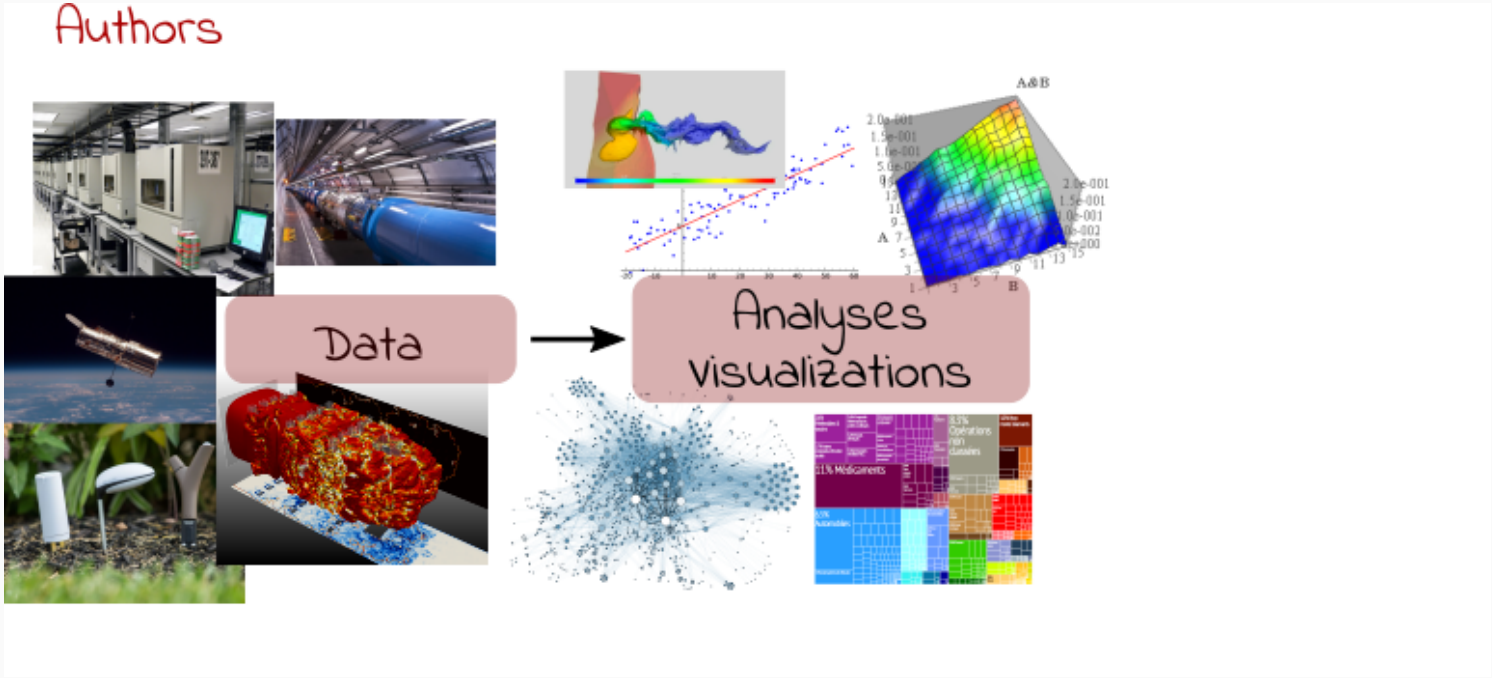

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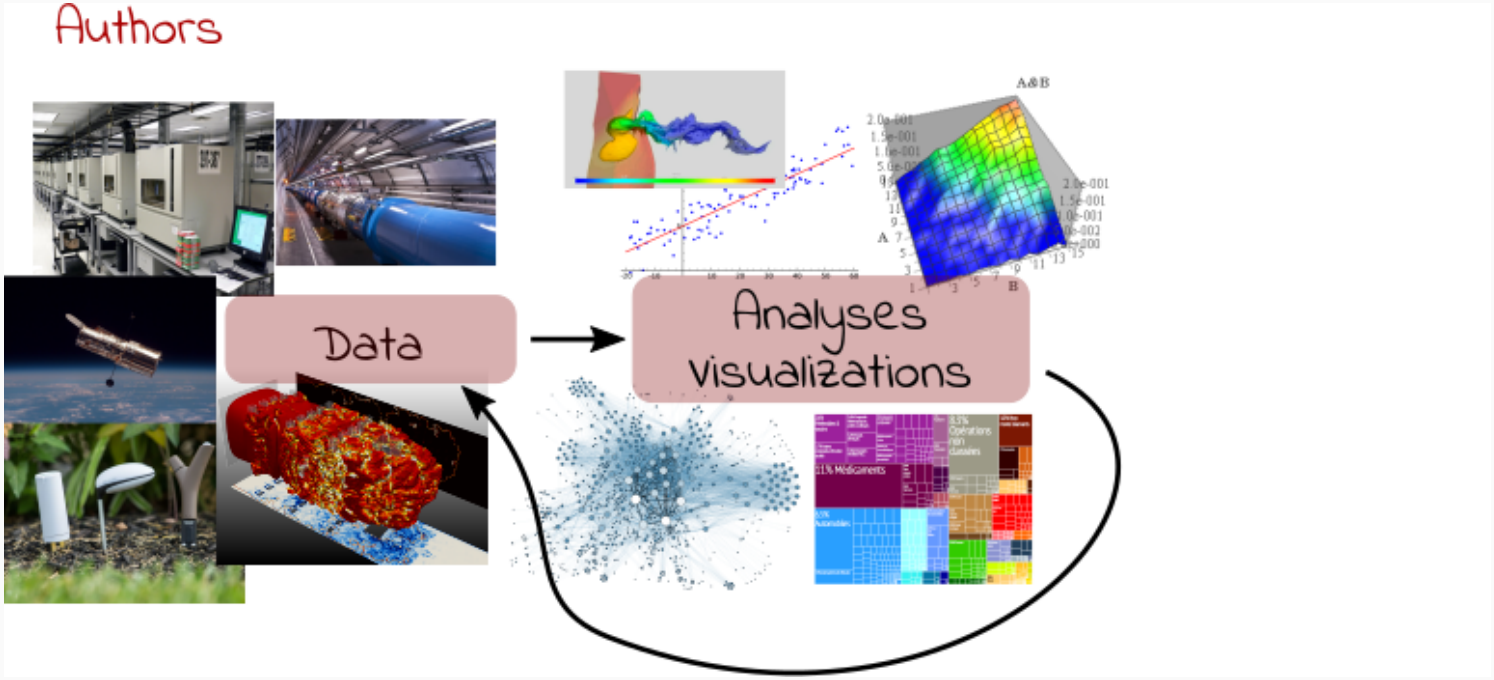

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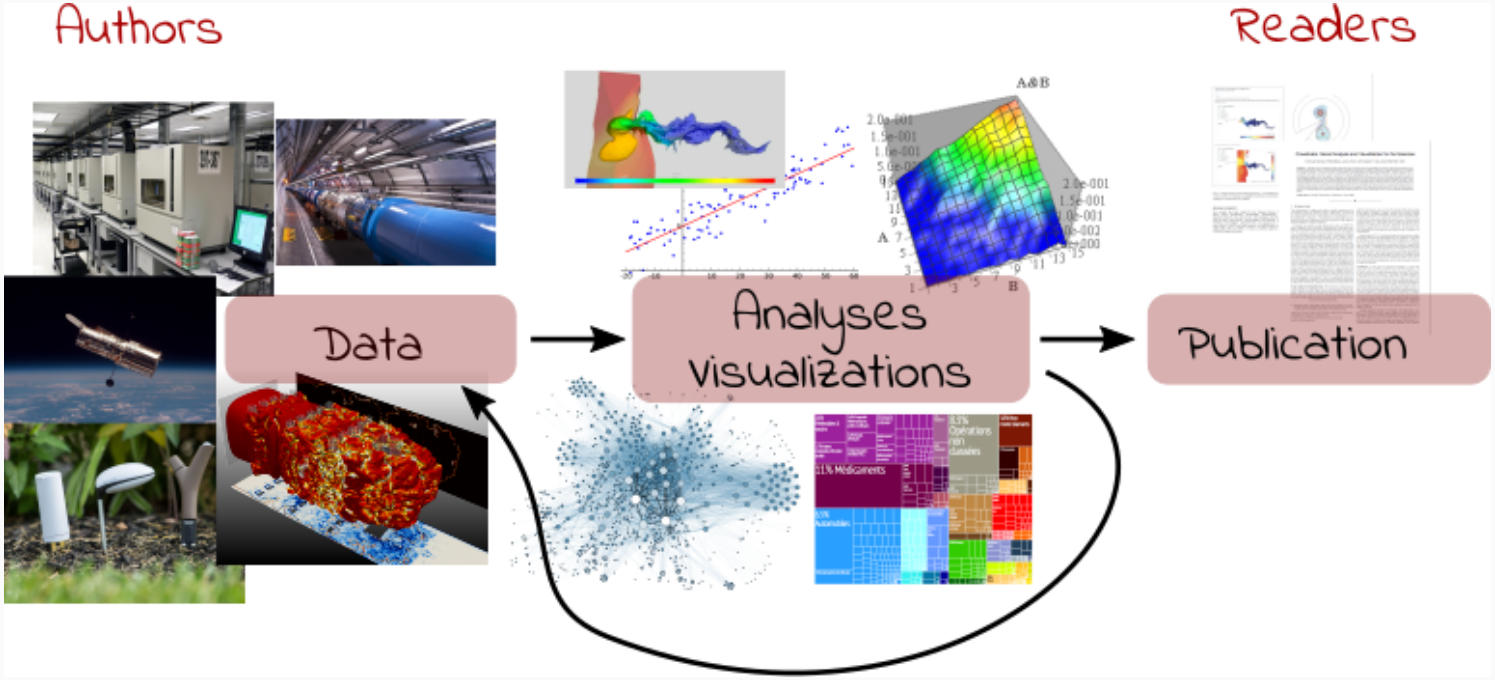

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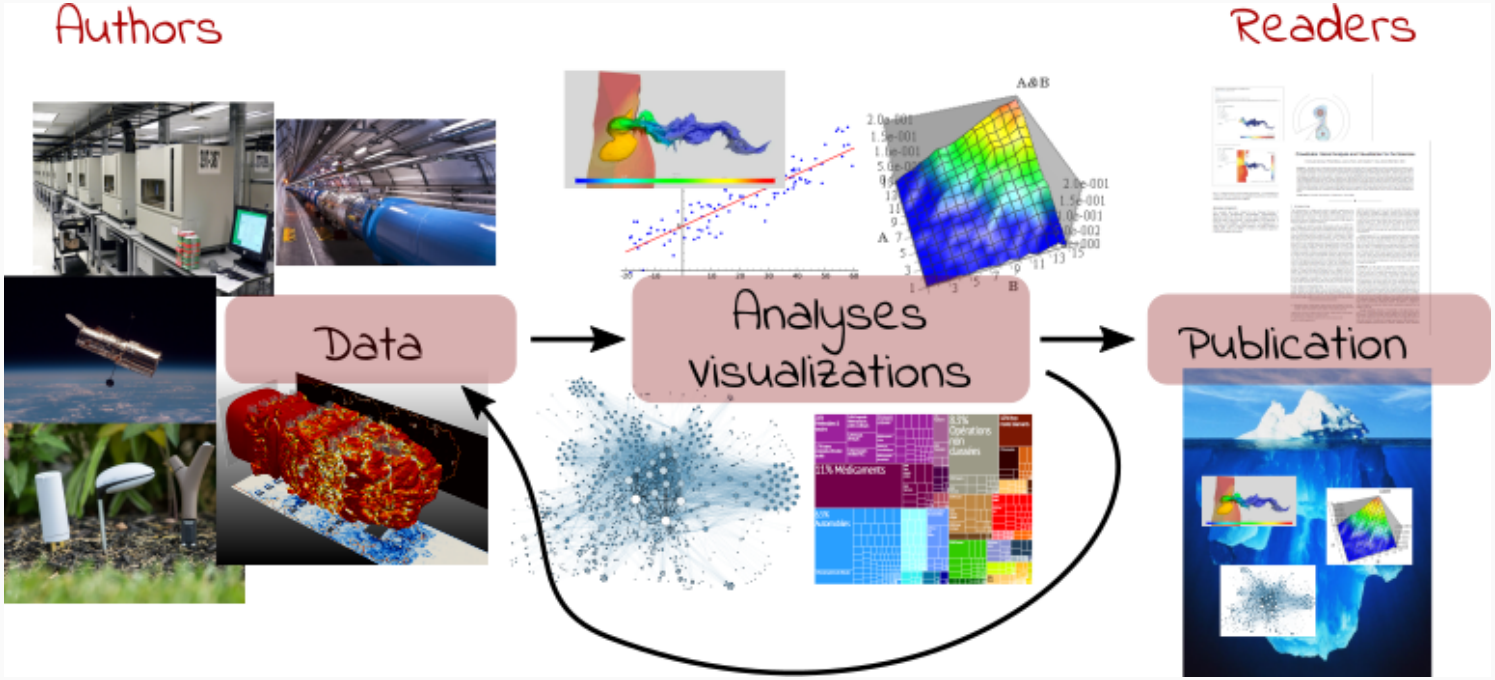

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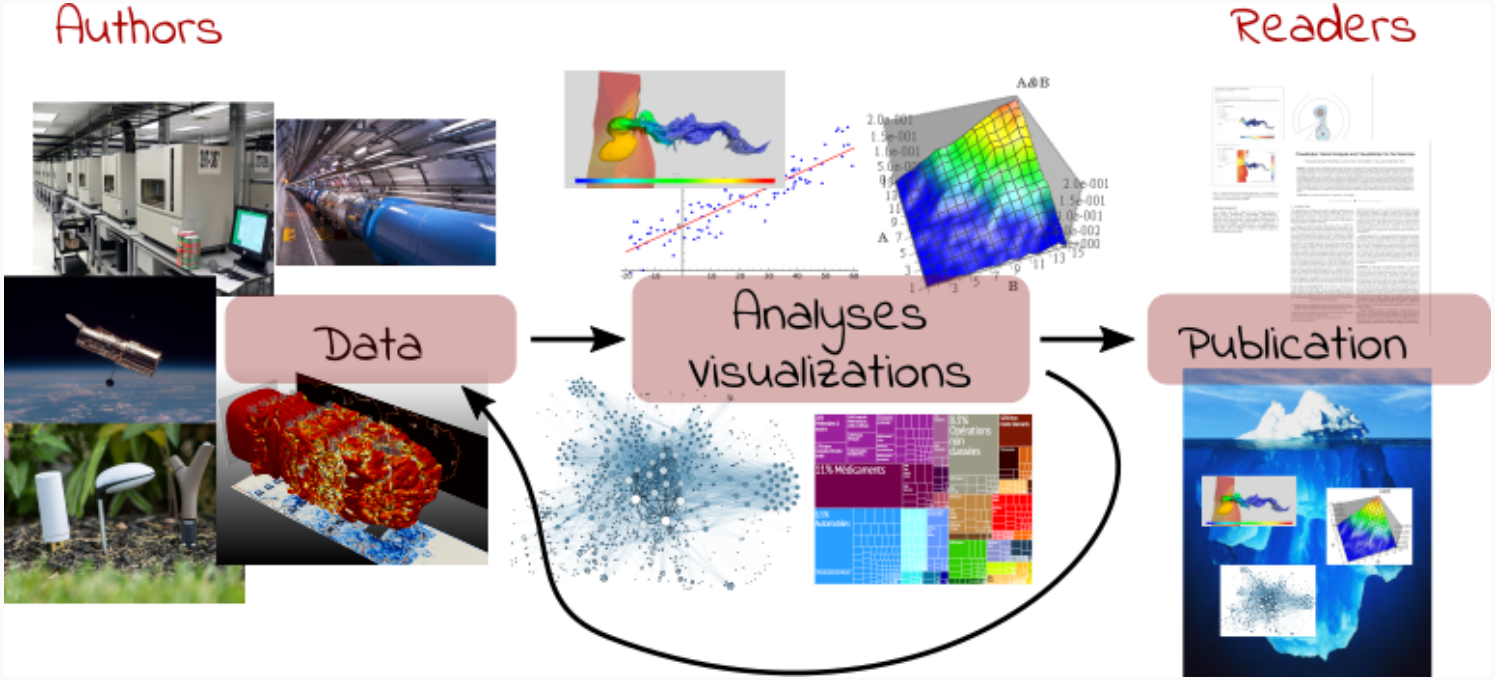

Reproducible Research = Bridging the Gap by working Transparently

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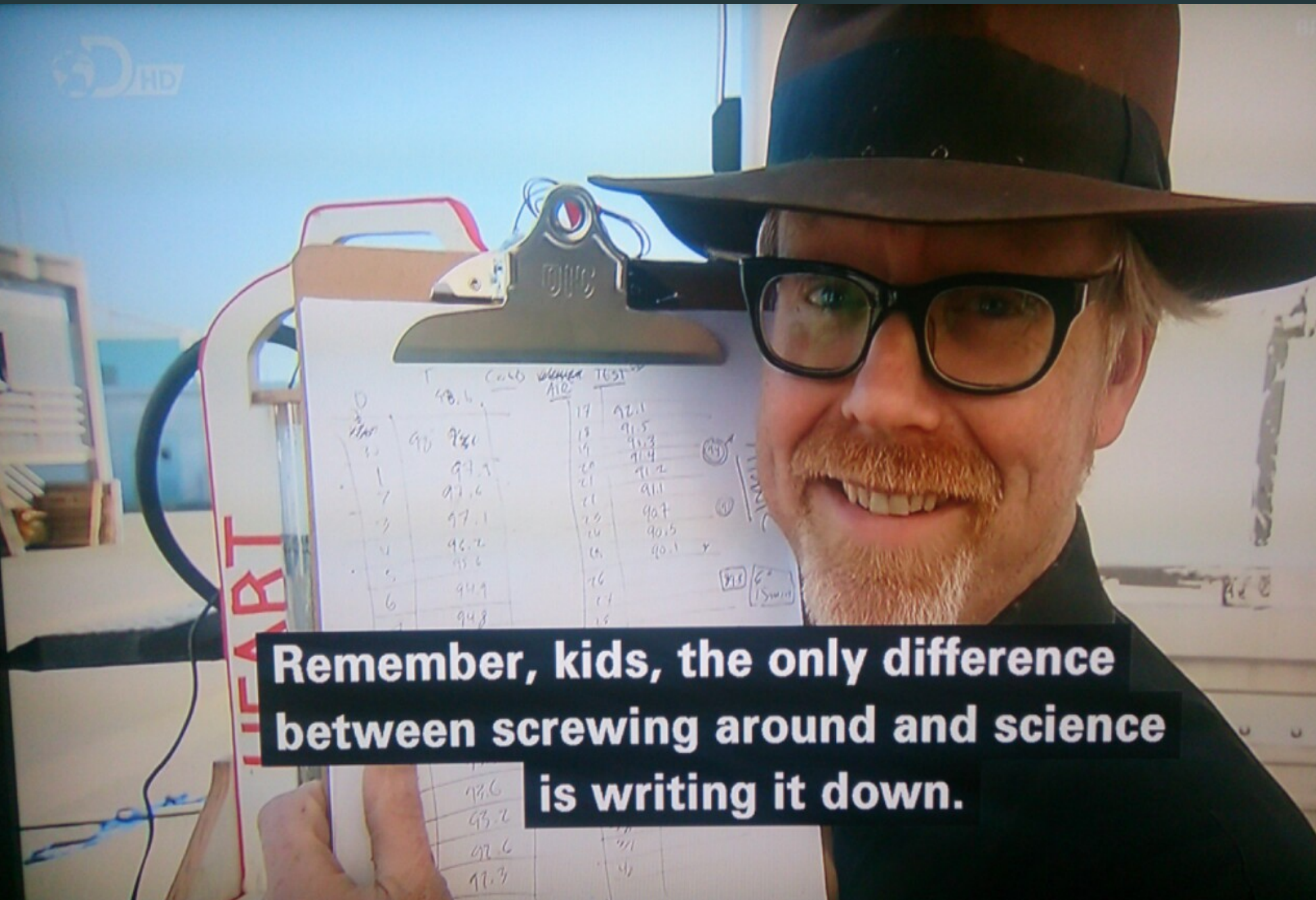
Tool 2: Electronic Notebooks



Taking notes

Org-mode and Markdown two simple text formats

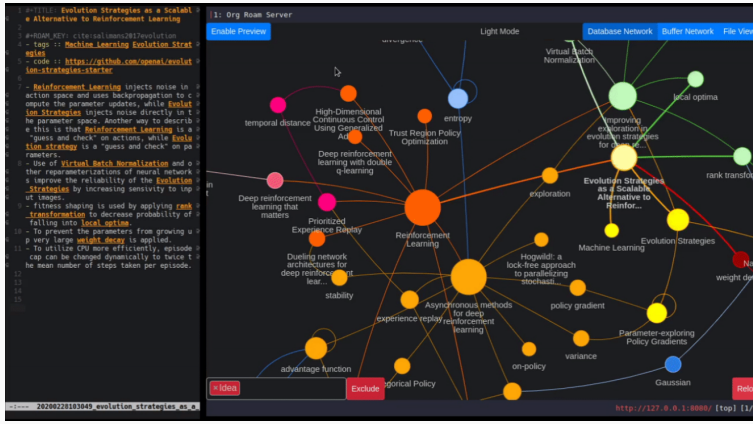
- simple formatting and export to more elaborate formats
- Hyperlinks, images, code, etc.

Journal structure

- My journal/notebook (single org file)
- Tom Cornebize's journal (single org file + Jupyter notebooks)

Zettelkasten possible structure

- Org-roam, Zettler, Roam, Obsidian, ...
- Architects, librarians, gardeners



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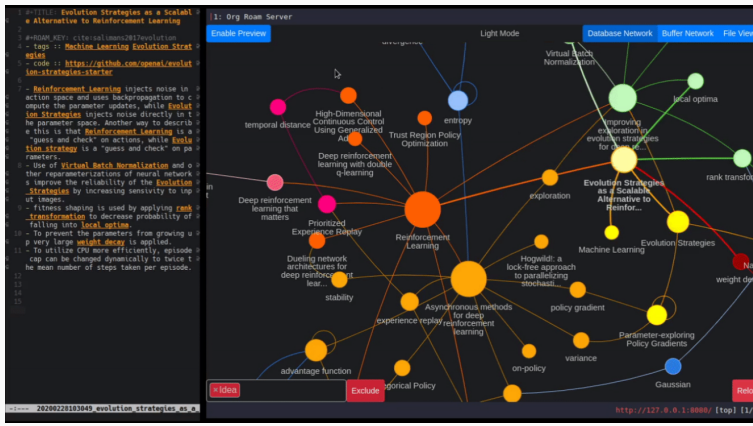

My recommendations: Do not use a fancy cloud-based proprietary tool

- Simple open source text-based format
- Control versions and backup yourself (e.g., using gitlab, github)
- Single location if possible
- Annotate (tags in a journal, links in a Zettelkasten)

Conclusion

Reproducible Research = Rigor and Transparency

Good research requires time and resources

1. **Train yourself and your students**: RR, statistics, experiments
   - Beware of checklists and norms Understand what's at stake

MOOC Reproducible Research: Methodological principles for a transparent science, Inria Learning Lab

- Konrad Hinsen, Christophe Pouzat
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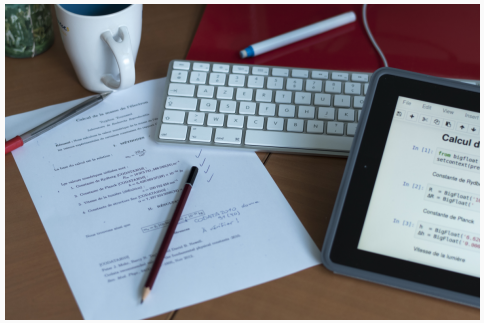

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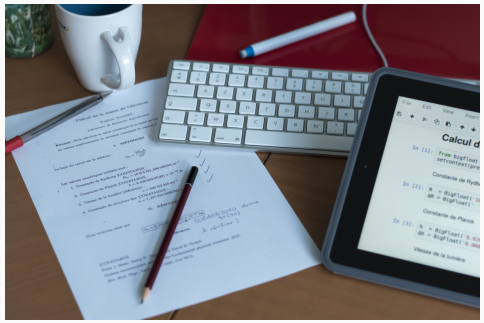

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MOOC "Advanced RR" planned for Jan. 2024

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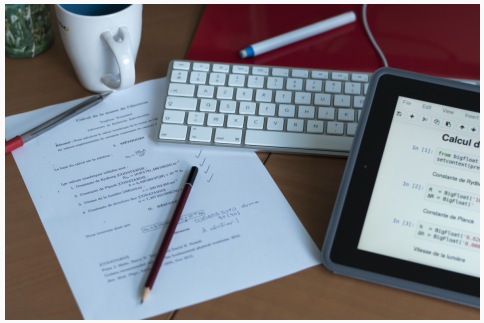

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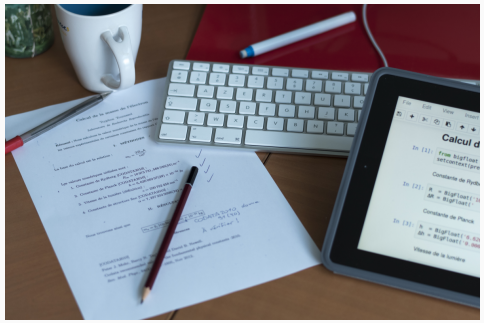

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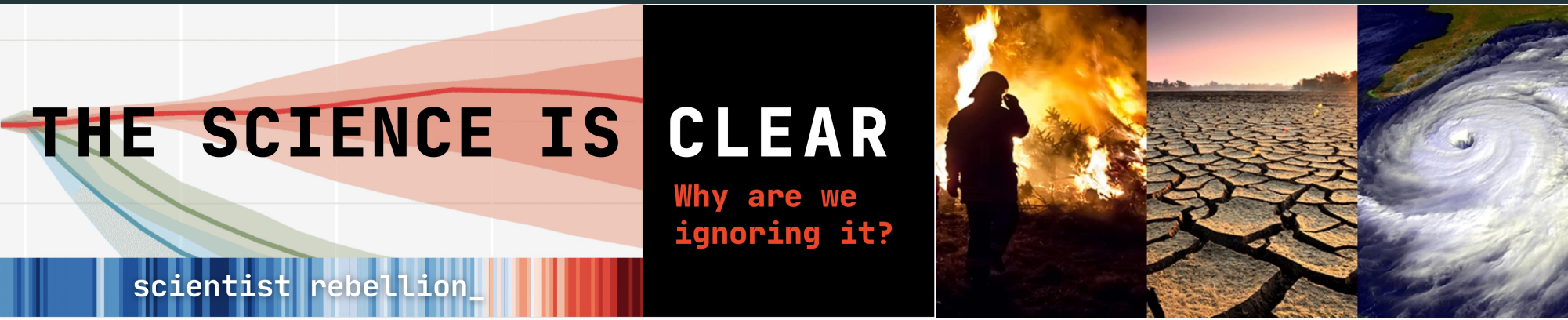
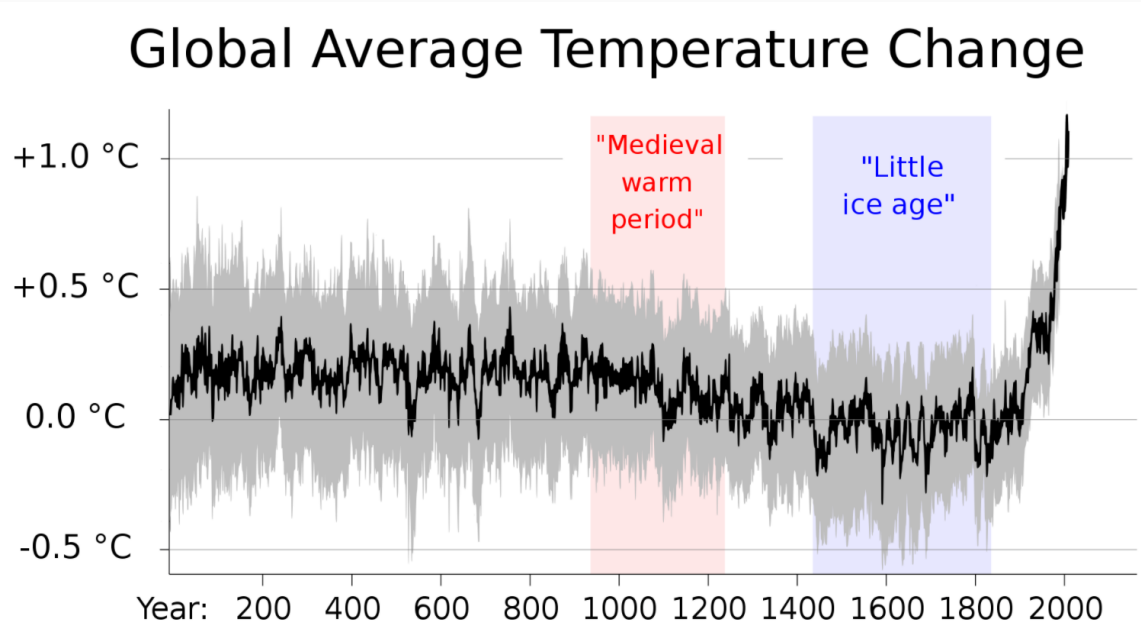
The Elephant in the Room: Climate Change

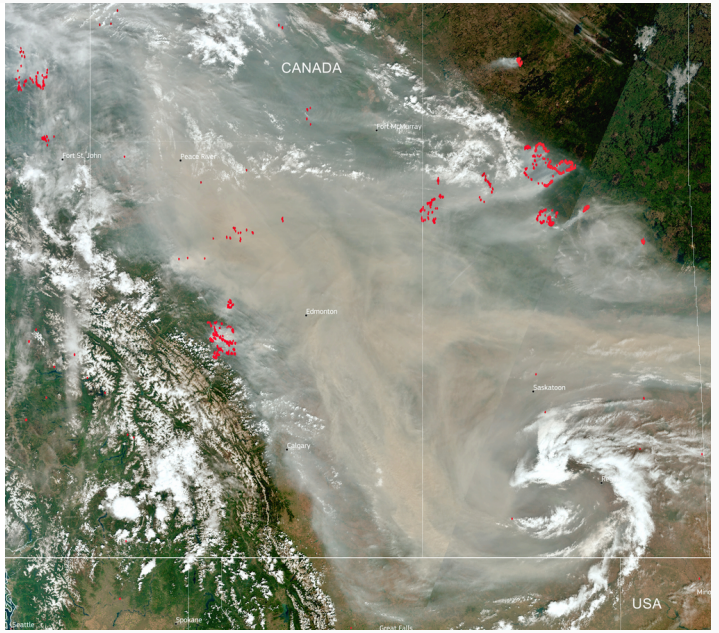


IPCC, IPBES, https://climate.nasa.gov/

1. Global climate change is **not** a future problem

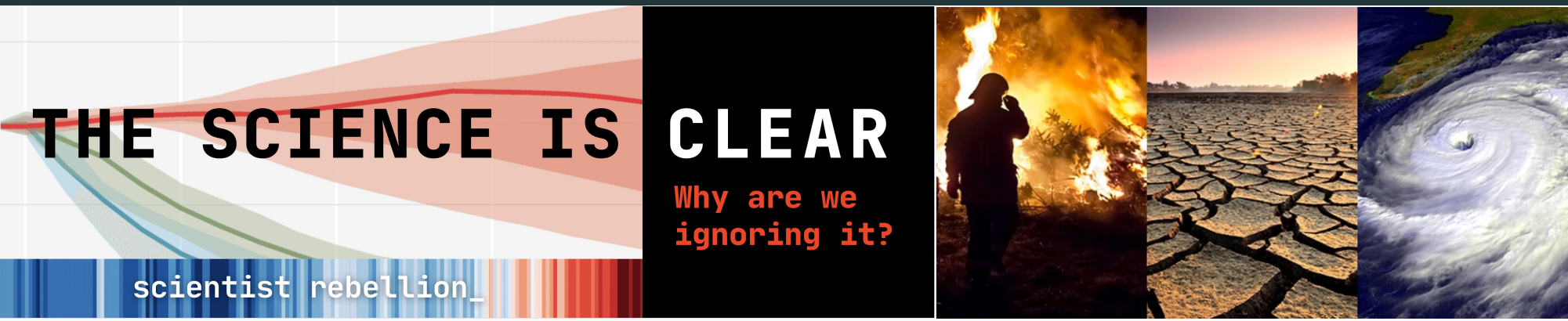


https://en.wikipedia.org/wiki/Global_temperature_record



2023 Alberta wildfires (> 1 Mha)

The Elephant in the Room: Climate Change



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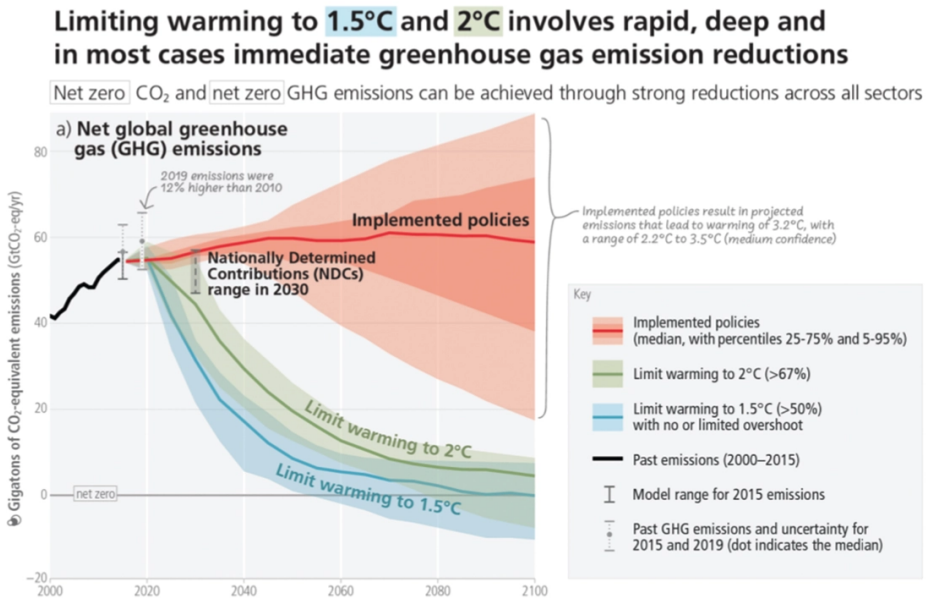
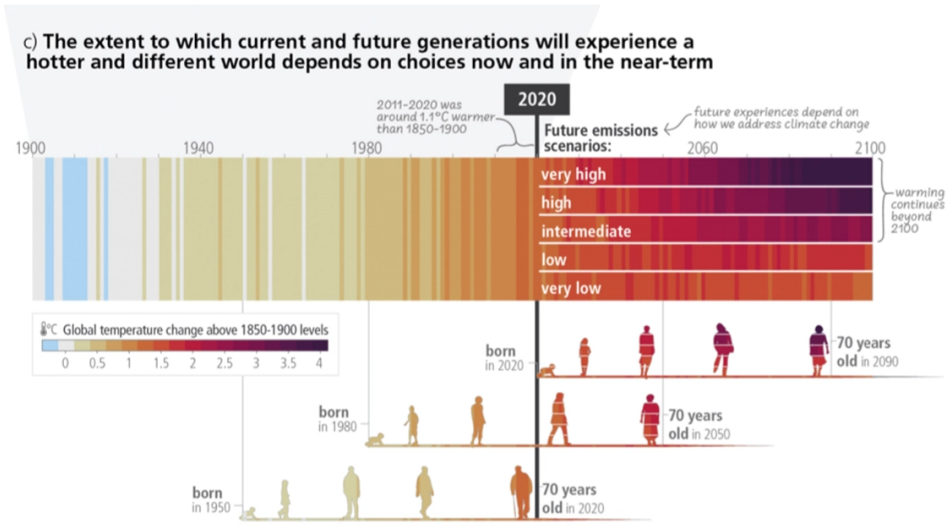
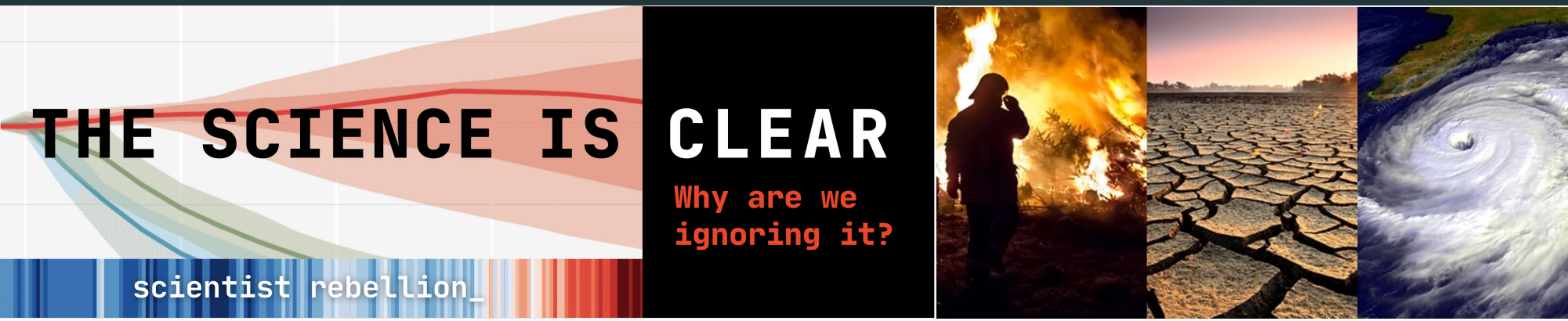




Paris Agreement'15 ∼ Net Zero by 2050

Latest IPCC report

The Elephant in the Room: Climate Change



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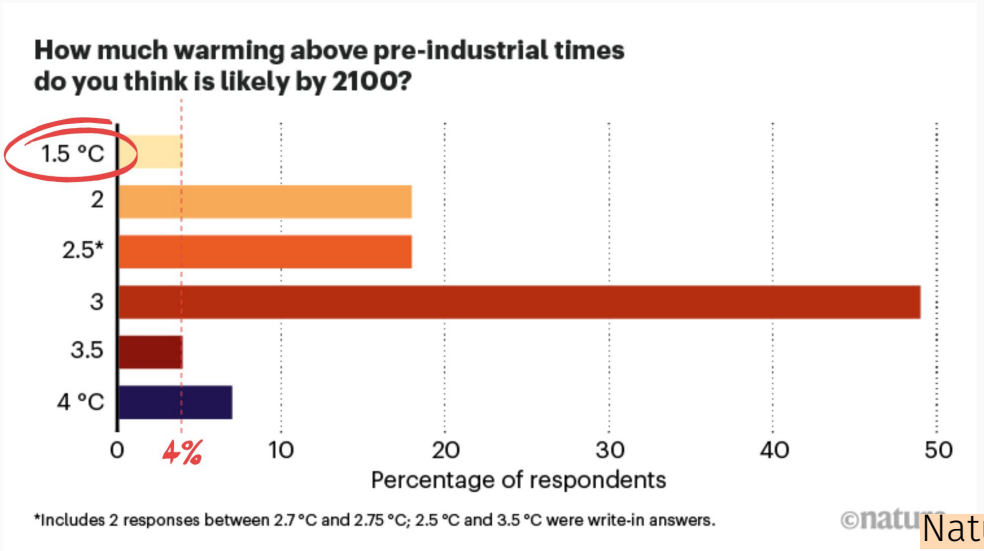
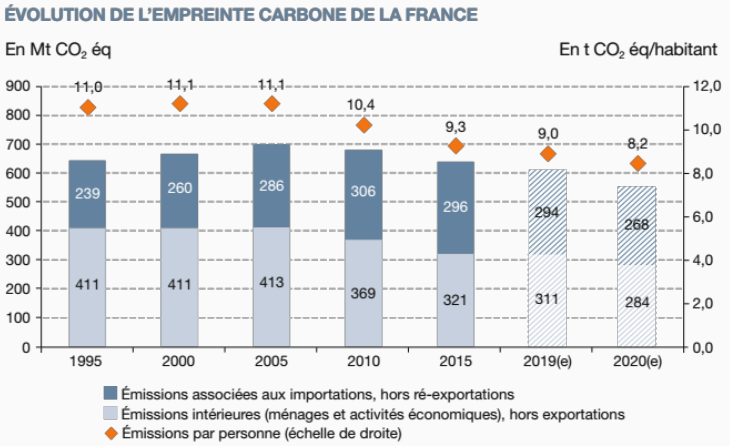
1. Global climate change is **not** a future problem
2. It is **entirely** due to human activity
3. *9 out of 10 IPCC scientists believe overshoot is likely*

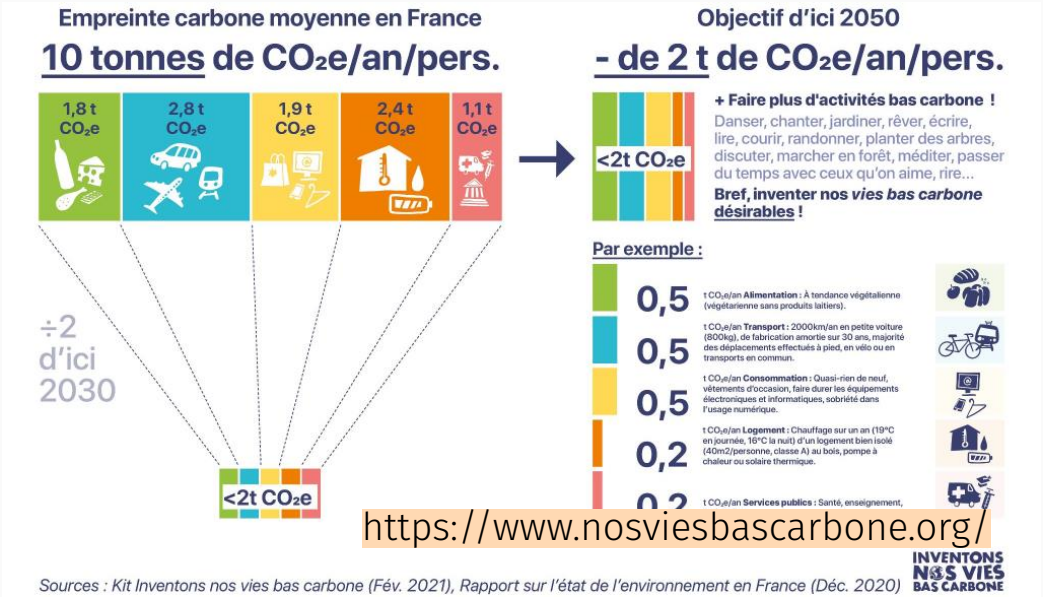


Nature survey, Nov. 2021

Put aside biodiversity loss, pollution, freshwater, land system change...



(e) = estimations.
Note : l'empreinte carbone porte sur les trois principaux gaz à effet de serre (CO_2, CH_4, N_2O). En 2021, la méthodologie a été ajustée afin de mieux tenir compte de l'évolution des coûts du pétrole brut, du gaz et du charbon ; l'ensemble de la série a ainsi été révisée, l'essentiel des ajustements portant sur les émissions importées de CH_4.
Champ : périmètre Kyoto (métropole et outre-mer appartenant à l'UE).
***Sources :** Citepa ; AIE ; FAO ; Douanes ; Eurostat ; Insee. Traitement : SDES, 2021*



Sources : Kit Inventons nos vies bas carbone (Fév. 2021), Rapport sur l'état de l'environnement en France (Déc. 2020)

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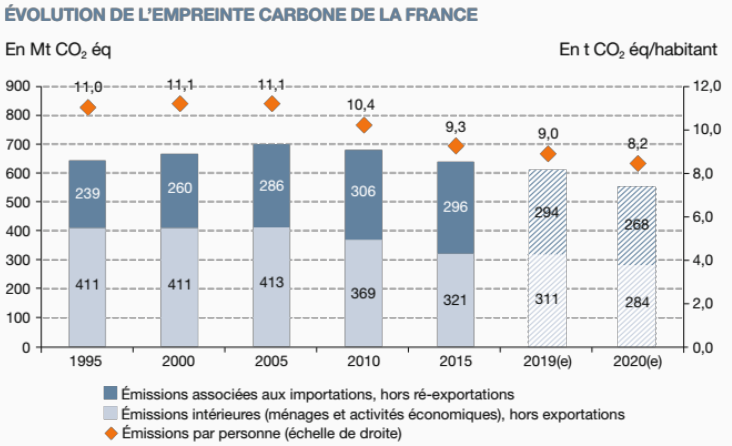

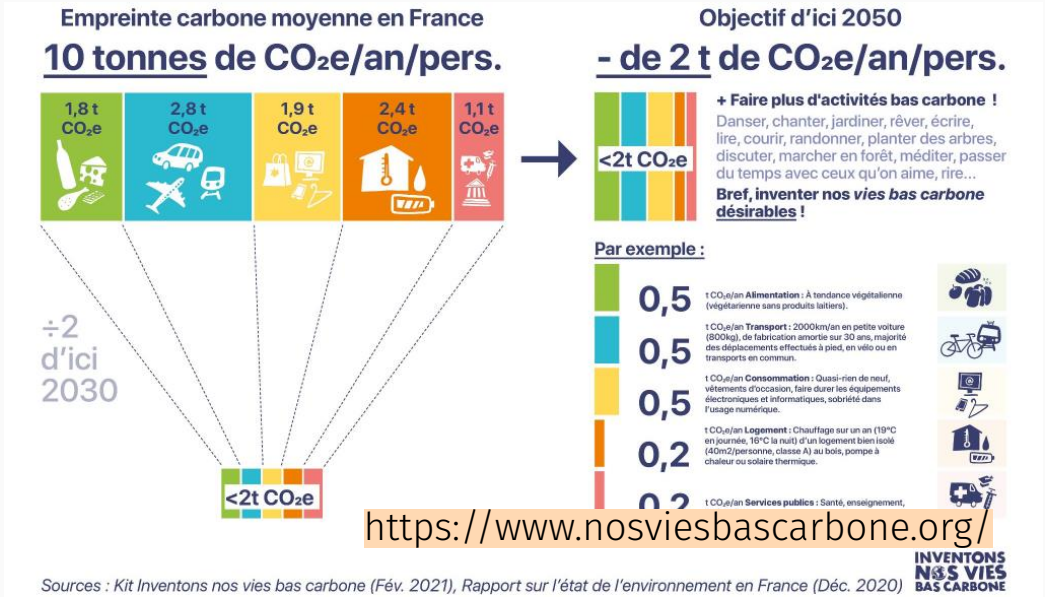

French government response

- *Verdissement de l'industrie: « pause » sur les normes environnementales*
- *Loi de programmation militaire (+41%)*
- *Nous devons préparer la France à une élévation de la température de 4 °C*
- Academia ? PEPR 5G, Cloud, NUMPEX, Quantique, IA, Agroécologie et numérique

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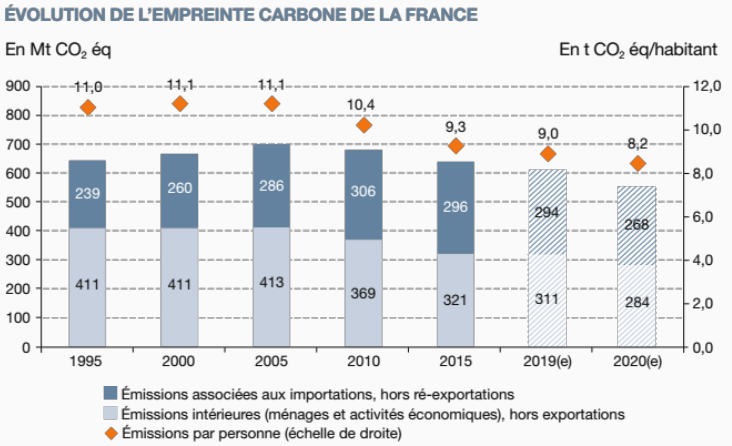

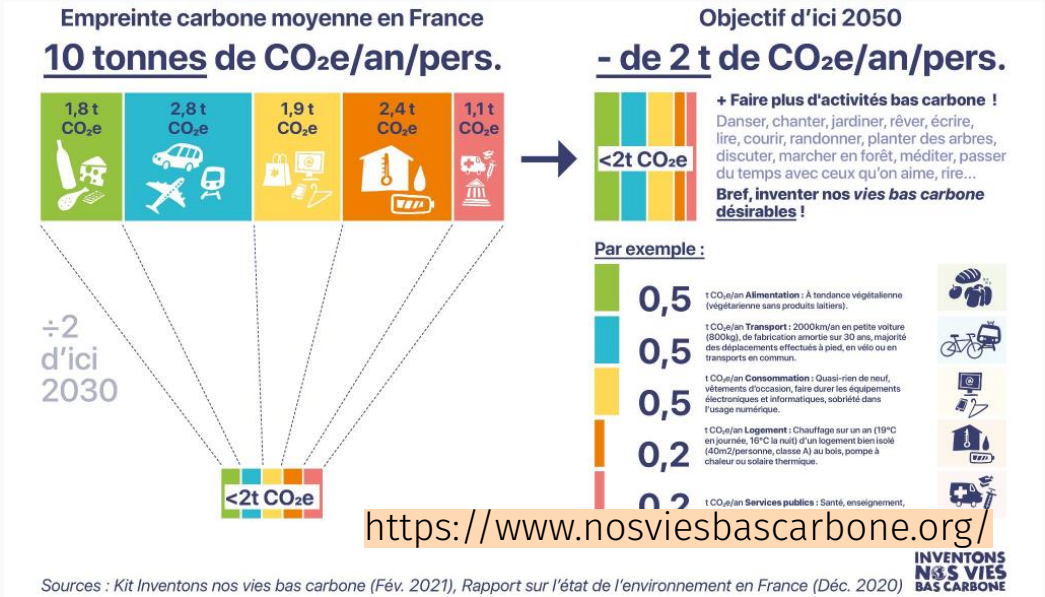

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~~Several~~ scenarios on the table

- What will research/CS look like/be used for in such a world?
- Energy optimization/saving ≠ sobriety and frugality

Other nightmares and tools

Nightmare 1: Fighting Software Environments Nightmare

What is hiding behind a simple

```
1 import matplotlib
```

```
Package: python3-matplotlib
Version: 2.1.1-2
Depends: python3-dateutil, python-matplotlib-data (>= 2.1.1-2),
python3-pyparsing (>= 1.5.6), python3-six (>= 1.10), python3-tz,
libjs-jquery, libjs-jquery-ui, python3-numpy (>= 1:1.13.1),
python3-numpy-abi9, python3 (<< 3.7), python3 (>= 3.6~),
python3-cycler (>= 0.10.0), python3:any (>= 3.3.2-2~), libc6 (>=
2.14), libfreetype6 (>= 2.2.1), libgcc1 (>= 1:3.0), libpng16-16 (>=
1.6.2-1), libstdc++6 (>= 5.2), zlib1g (>= 1:1.1.4)
```

Nightmare 1: Fighting Software Environments Nightmare

What is hiding behind a simple

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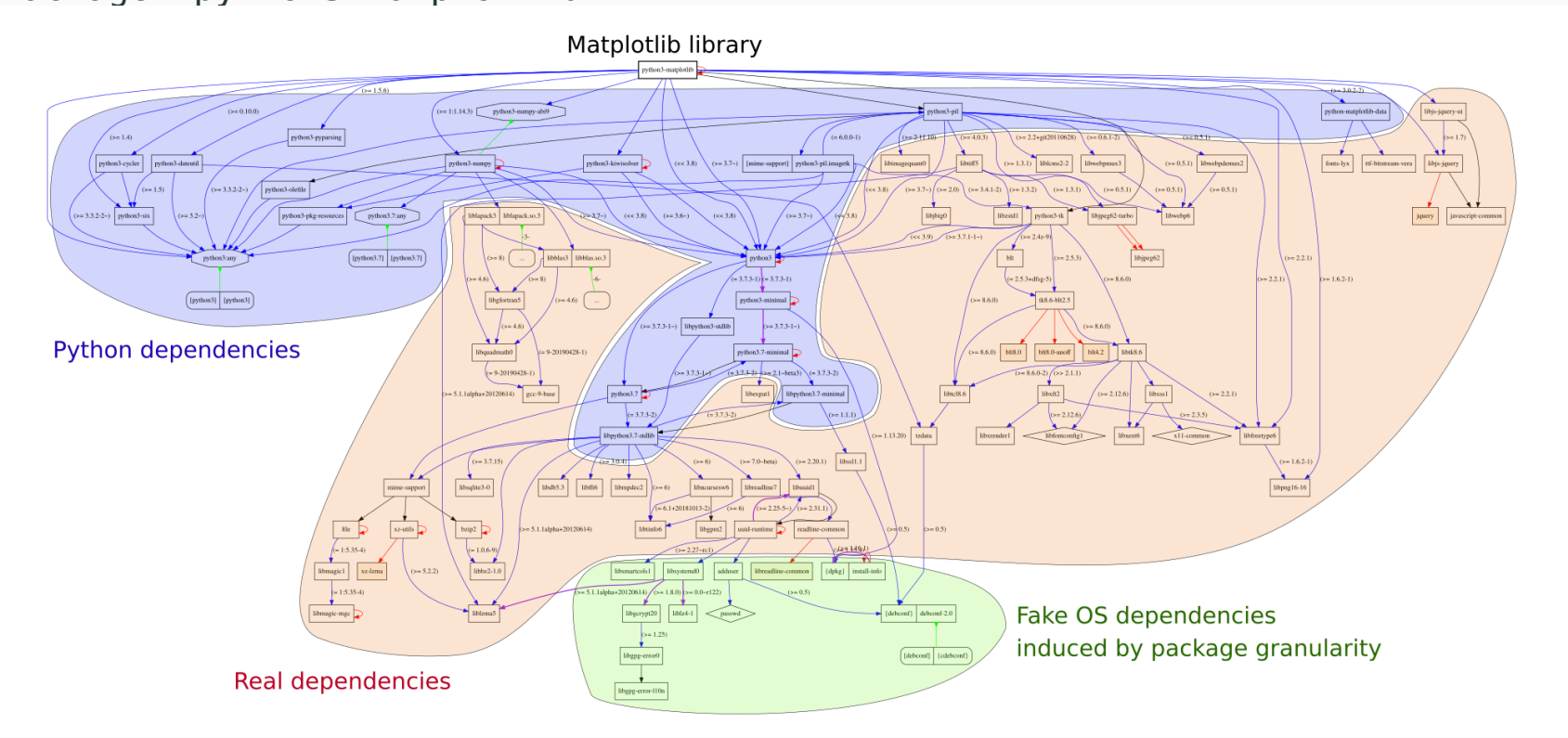
`Package: python3-matplotlib`



Nightmare 1: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

```
python2 -c "print(10/3)"
python3 -c "print(10/3)"
```

```
3
3.3333333333333335
```

Nightmare 1: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

```
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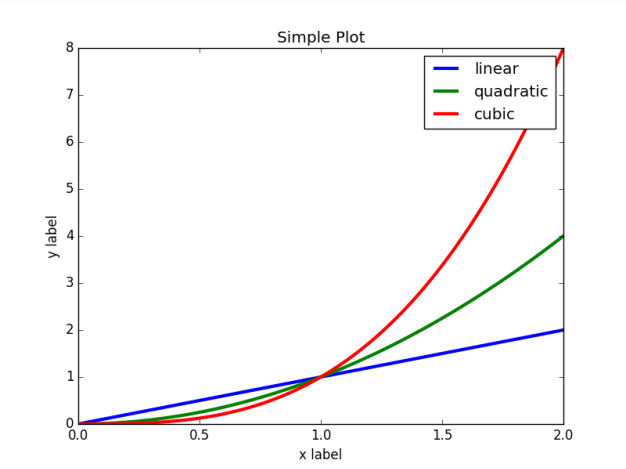
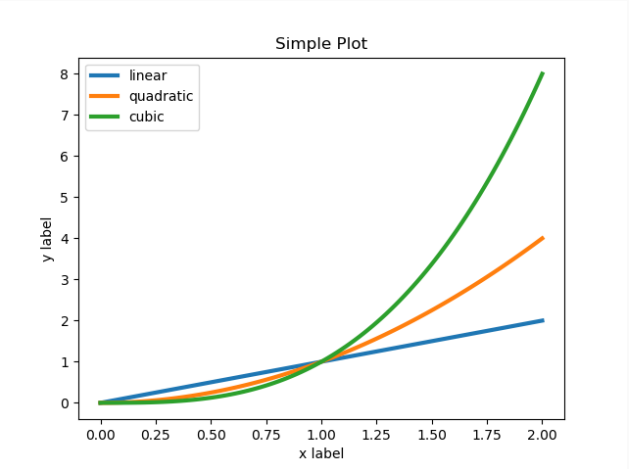
python3 -c "print(10/3)"
```





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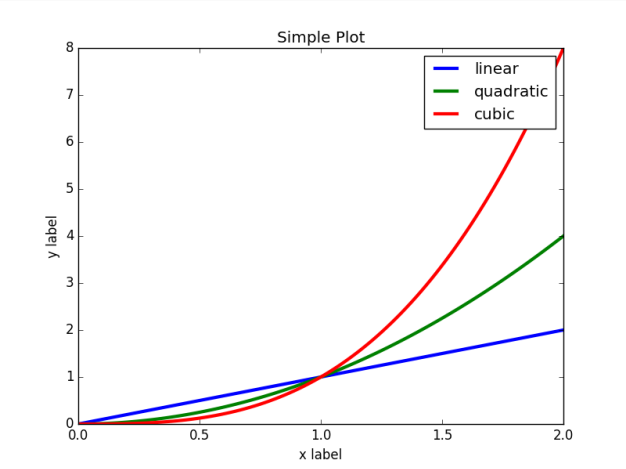

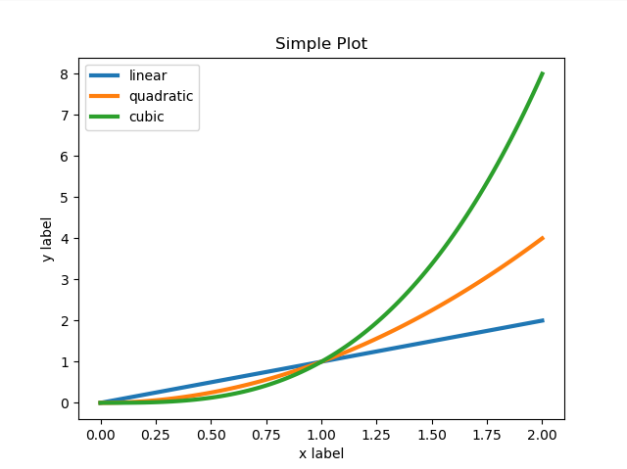

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Nightmare 1: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

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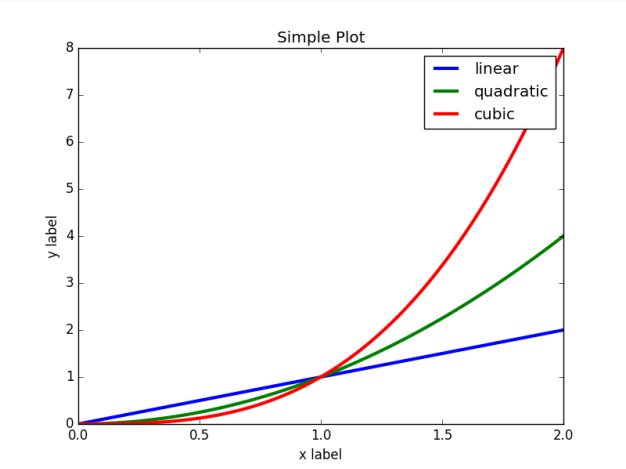

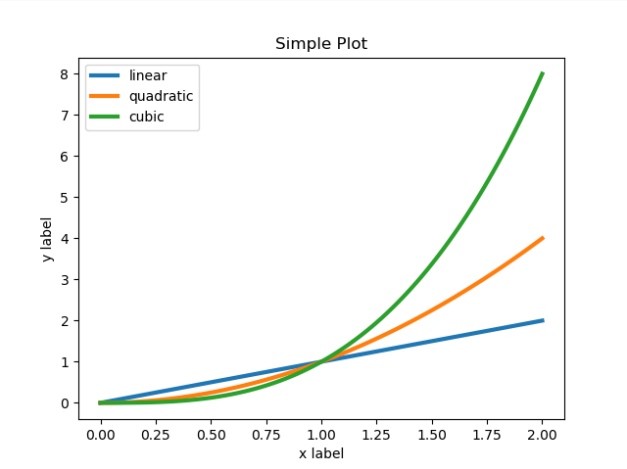

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ReproZip

Guix

Nightmare 2: Fighting Information Loss with Archives

D. Spinellis. *The Decay and Failures of URL References*. CACM, 46(1), Jan 2003.

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Software Archive Software Heritage


or  = awesome collaborations ≠ archive

That's all Folks!