Reproducibility Crisis and Open Science

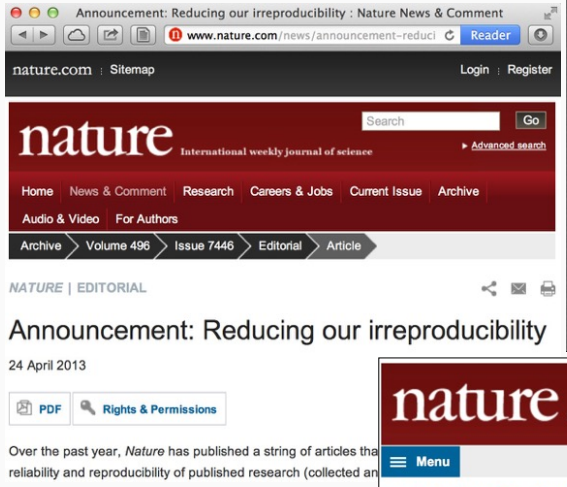
Arnaud Legrand

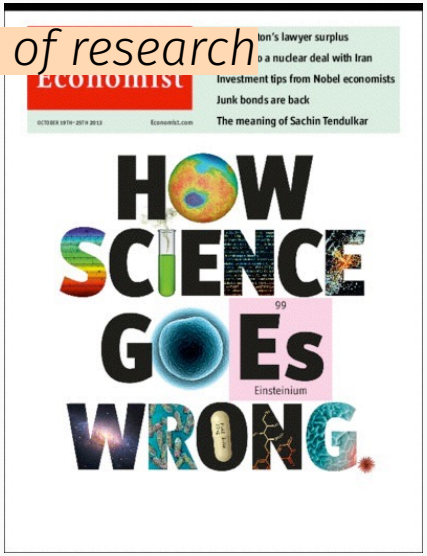
UGA Université Grenoble Alpes — cnrs — Inria informatics mathematics — LIG

Séminaire RR, Grenoble, April 2021

Public Evidence for a Lack of Reproducibility

- J.P. Ioannidis. *Why Most Published Research Findings Are False* PLoS Med. 2005.
- *Lies, Damned Lies, and Medical Science*, The Atlantic. Nov, 2010
- *Reproducibility: A tragedy of errors*, Nature, Feb 2016.
- Steen RG, *Retractions in the scientific literature: is the incidence of research fraud increasing?*, J. Med. Ethics 37, 2011





Courtesy V. Stodden, SC, 2015

Newsworthy Stories about Scientific Misconduct

Dong-Pyou Han Assistant professor, Biomedical sciences, Iowa State University, 2013

Falsified blood results to make it appear as though a vaccine exhibited anti-HIV activity

- Han and his team received ≈ $19 million from NIH
- 1 retracted publication and resignation of university. Sentenced in 2015 to 57 months imprisonment for fabricating and falsifying data in HIV vaccine trials. $7.2 million!

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Dieterik Stapel Professor, Social Psychology, Univ. Amsterdam, 2011

I failed as a scientist. I adapted research data and fabricated research. Not once, but several times, not for a short period, but over a longer period of time. [..] I am aware of the suffering and sorrow that I caused to my colleagues... I did not withstand the pressure to score, to publish, the pressure to get better in time. I wanted too much, too fast. In a system where there are few checks and balances, where people work alone, I took the wrong turn.

58 retracted publications

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Brian Wansink Professor, Psychological Nutrition, Cornell, 2016

I gave her a data set of a self-funded, failed study which had null results. I said "This cost us a lot of time and our own money to collect. There's got to be something here we can salvage because it's a cool (rich & unique) data set." I told her what the analyses should be. [..] Every day she came back with puzzling new results, and every day we would scratch our heads, ask "Why," and come up with another way to reanalyze the data with yet another set of plausible hypotheses

17 retracted publications

Scientific Misconduct? What are the consequences ?

Reinhart and Rogoff Professors of Economics at Harvard

> *gross debt [..] exceeding 90 percent of the economy has a significant negative effect on economic growth* – *Growth in a Time of Debt (2010)*
>
> *While using RR's working spreadsheet, we identified coding errors, selective exclusion of available data, and unconventional weighting of summary statistics.* – *2013: Herndon, Ash and Pollin*
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> *For 3 years, austerity was not presented as an option but as a necessity.* – *2013: Paul_Krugman*

At least, a scientific debate has been possible.

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Bad science is **deleterious**

- It is used to backup stupid politics, it affects people's life, ...
- It blurs the frontier between scientists and crooks

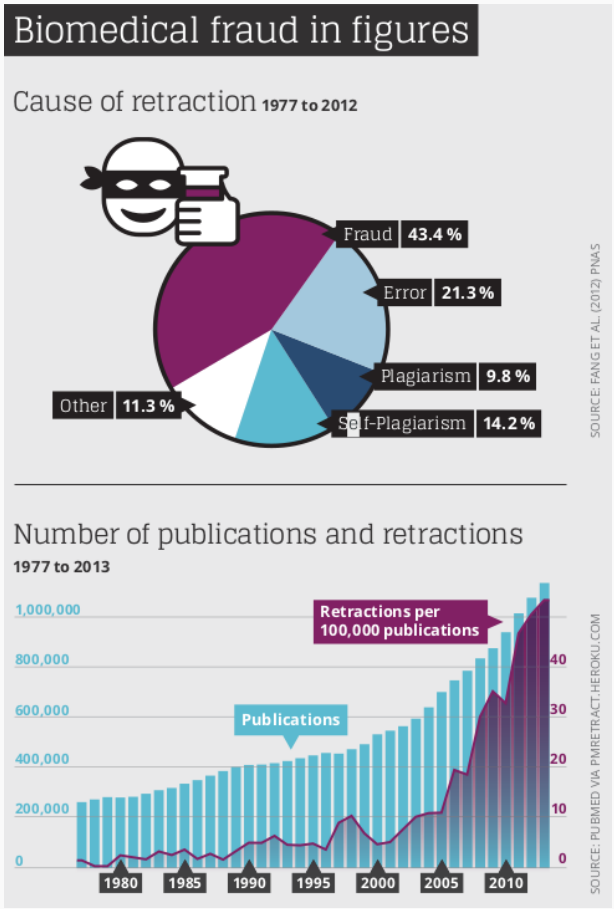
Media attention inflates **conspiracy** opinions ☹

- *Scientific result are worthless.*
- *Scientists can't even agree with each others on economy/climate/vaccine/5G/...*
- *Stop the scientific dictatorship/lobby!*

A Credibility Crisis?

How so? Why now? Why is this important? What can we do about it?

The Battle against Scientific Fraud in the CNRS International Magazine

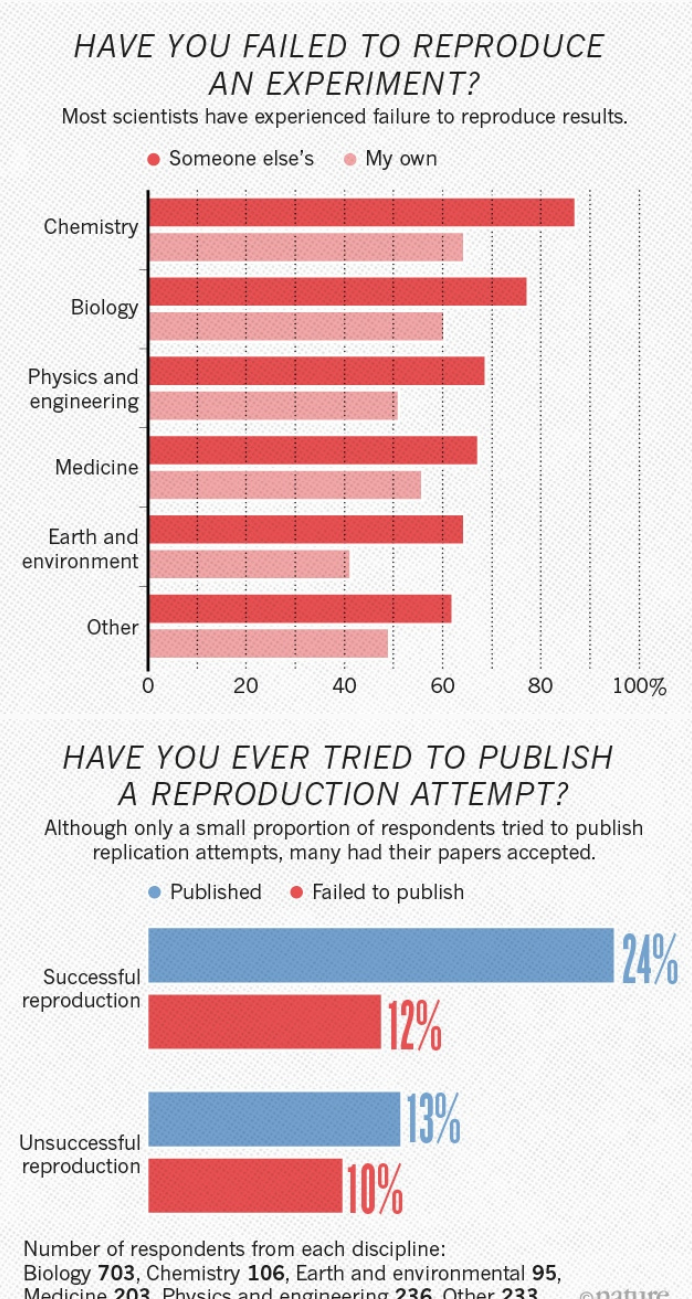


Galileo (data fabrication), **Ptolemy** (plagiarism), **Mendel** (data enhancement), **Pasteur** (rigorous but hid failures), ...

Scientific misconduct is obviously wrong but it's not new!

- Every domain has its black sheep
- The publish or perish pressure is a pain

A Reproducibility Crisis?



1,500 scientists lift the lid on reproducibility, Nature, May 2016

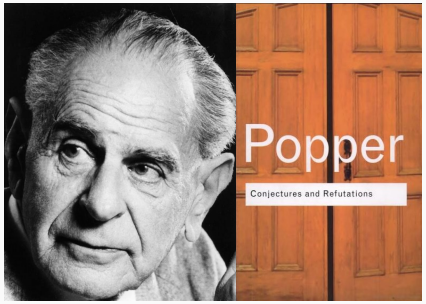
Methodological or technical causes

- The many biases (apophenia, confirmation, hindsight, experimenter, ...): bad designs
- Selective reporting, weak analysis (statistics, data manipulation mistakes, computational errors)
- Lack of information, code/raw data unavailable

Social causes

- Fraud, conflict of interest (pharmaceutic, ...)
- No incentive to reproduce/check our own work (afap), nor the work of others (big results!), nor to allow others to check (competition)
- Peer review does not scale: 1+ million articles per year!

Reproducibility of experimental results: the *hallmark of science*



1934: **Karl Popper** puts the notions of falsifiability and crucial experiment as the hallmark of science

- If no experiment can be set up to disprove your theory, it is not science
- Good experiments discriminate good theories from bad ones
- Non-reproducible single occurrences are of no significance to science

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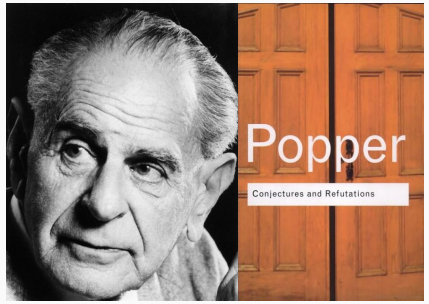

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An ideal rather than the norm

Popper's proposal works well for Physics from the 18th century but is not so simple for many other domains:

- Theory of evolution
- Spotting a SuperNova
- Particle Physics (a single LHC)
- Biology (every animal does not behave in the same way)
- Anthropology (impact on people from a remote culture)

Reproducibility: a *core value of science*

1. Universality: Science aims for objective findings, accessible to anyone

   Reproducibility acts as a Universality/Robustness control

2. Incremental: We build on each others work but everybody makes mistakes

   Methods, biases, ... How to discriminate sound ~~theories~~ experiments from bad ones? 😉

   Reproducibility acts as a Quality control

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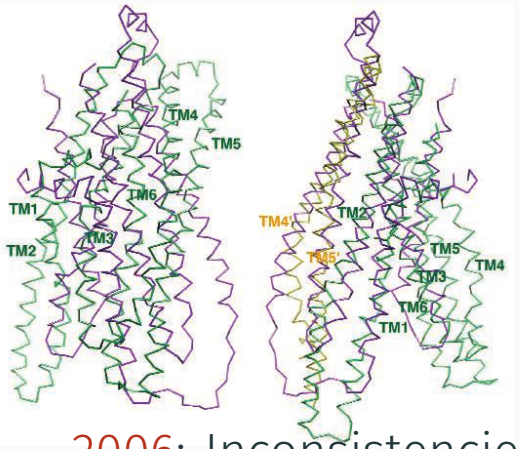
But, scientific practices have greatly evolved, in particular since we rely on computers

How computers broke science – and what we can do about it

– Ben Marwick, The conversation, 2015

How computers broke science



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He specialized in structures of multidrug resistant transporter proteins in bacteria: MsbA de Escheria Choli (Science, 2001), Vibrio cholera (Mol. Biology, 2003), Salmonella typhimurium (Science, 2005)

2006: Inconsistencies reveal a programming mistake

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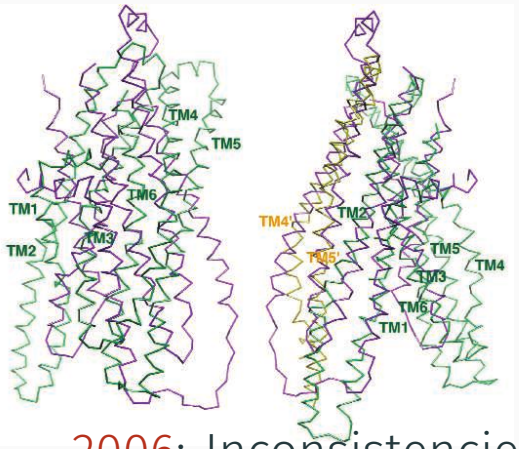
5 retractations that motivate improved software engineering practices in comp. biology

How computers broke science



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There is worse!

- The generalized and intensive use of spreadsheets (COVID tracing)
- Relying on black box statistical methods is infinitely easier than understanding them (Learning and Data Analytics frameworks = nuke)
- Numerical errors and software environment unawareness

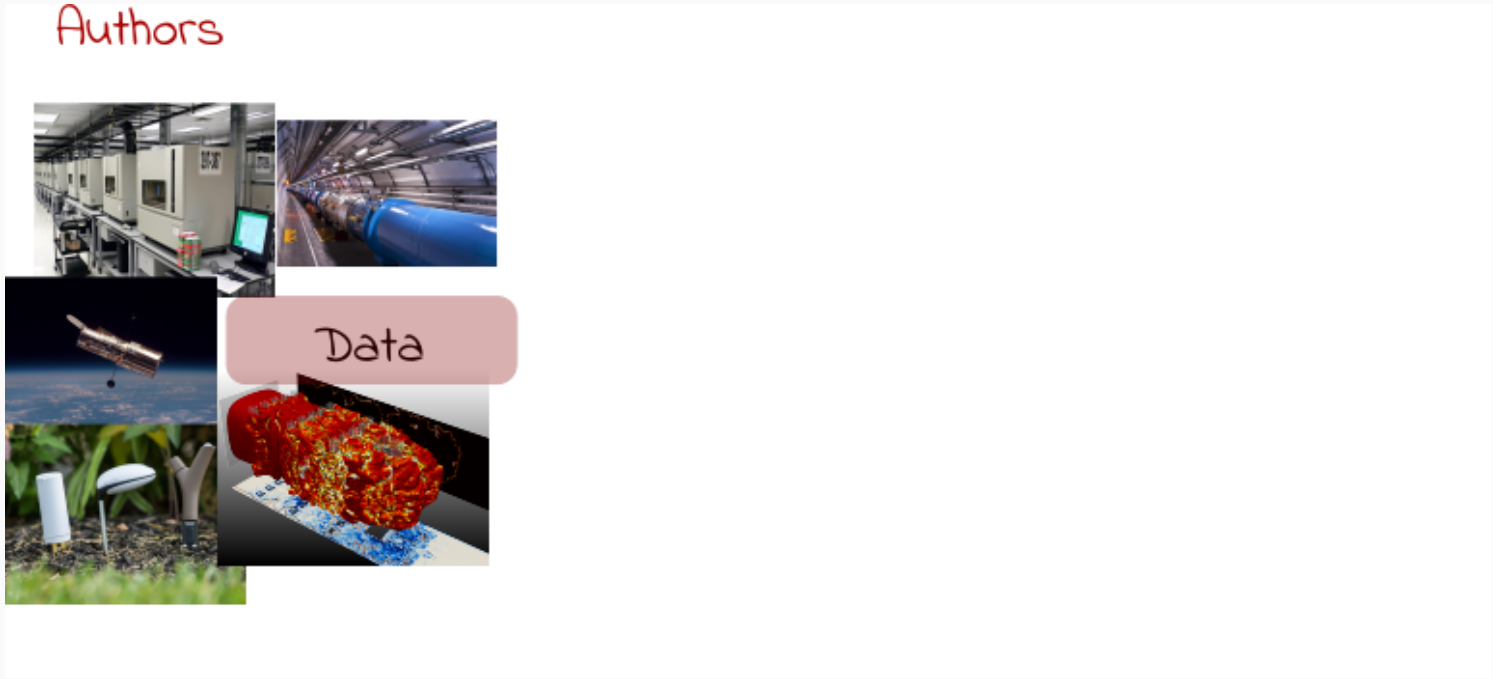
Different Reproducibility Concerns in Modern Science

Social Sciences, Oncology, ... methodology, statistics, pre-registration

Genomics software engineering, computational reproducibility, provenance

Computational fluid dynamics numerical issues

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



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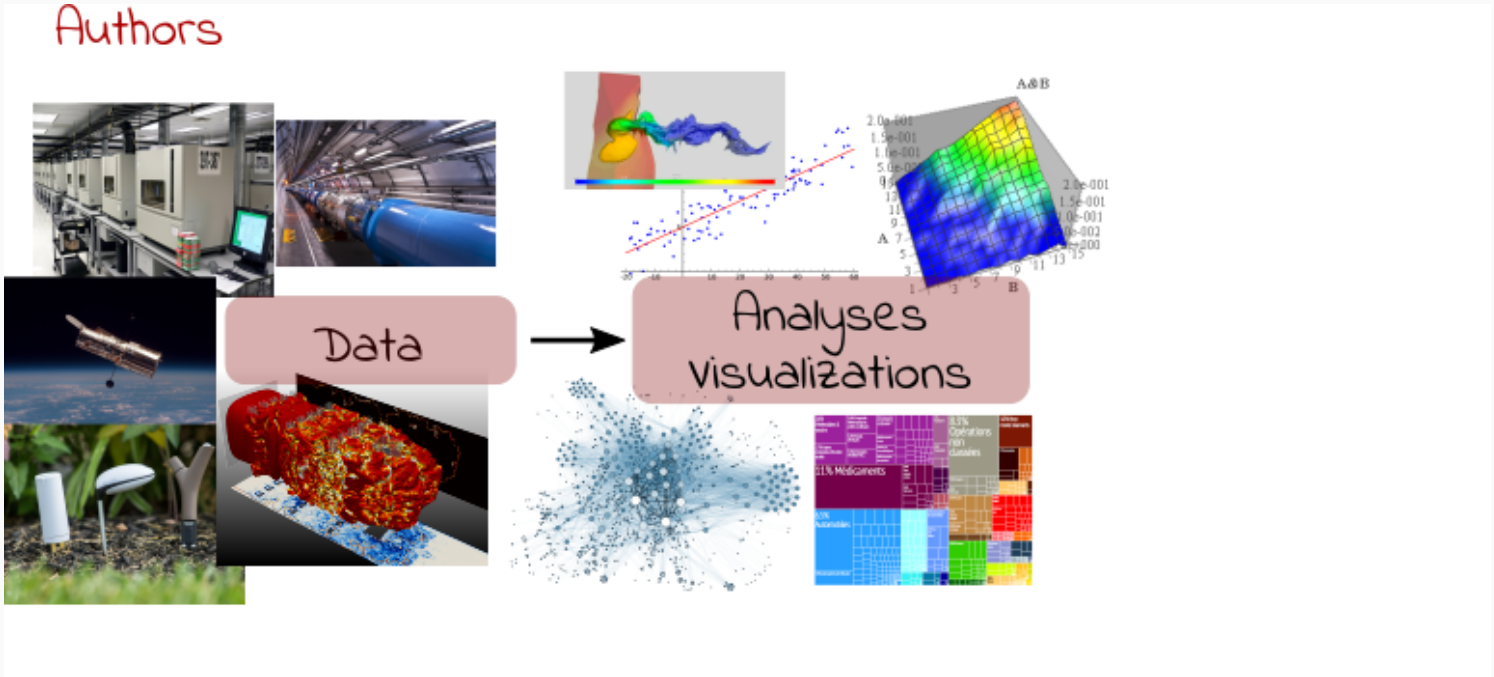

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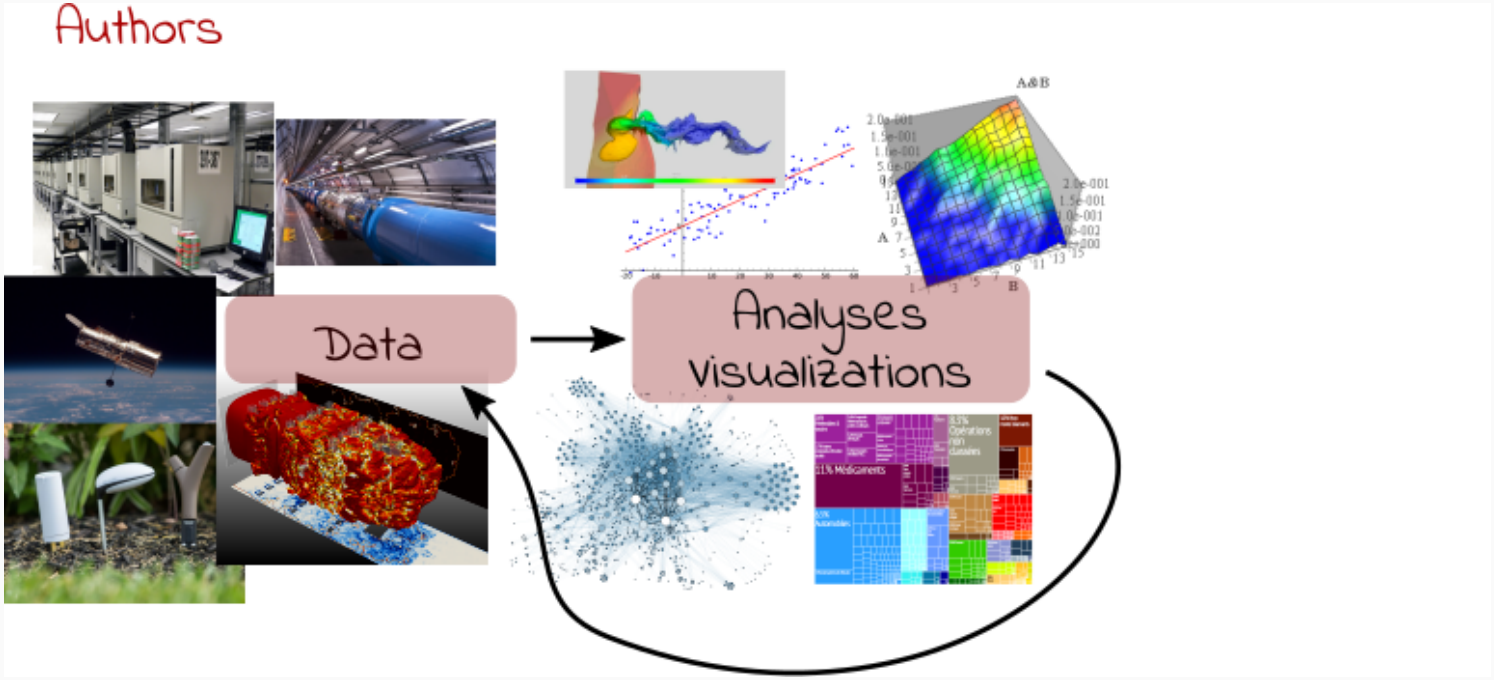

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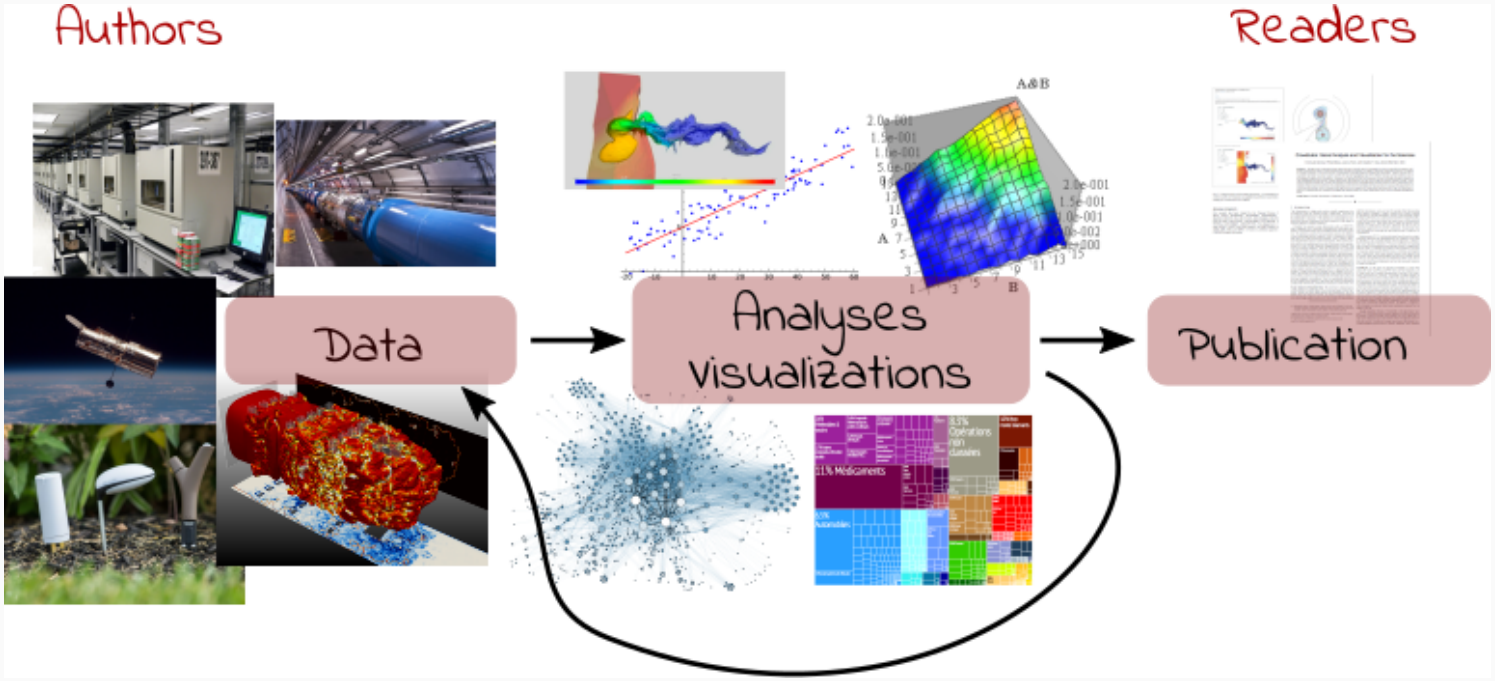

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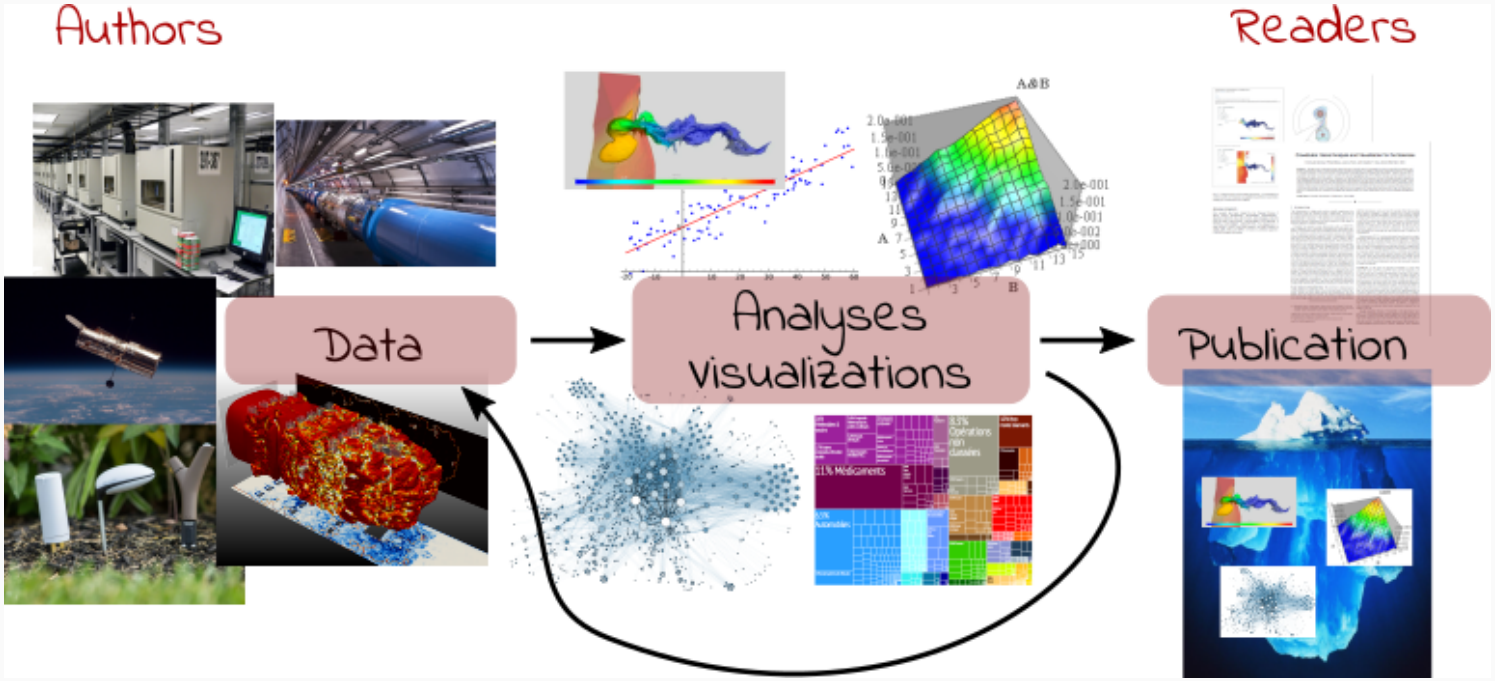

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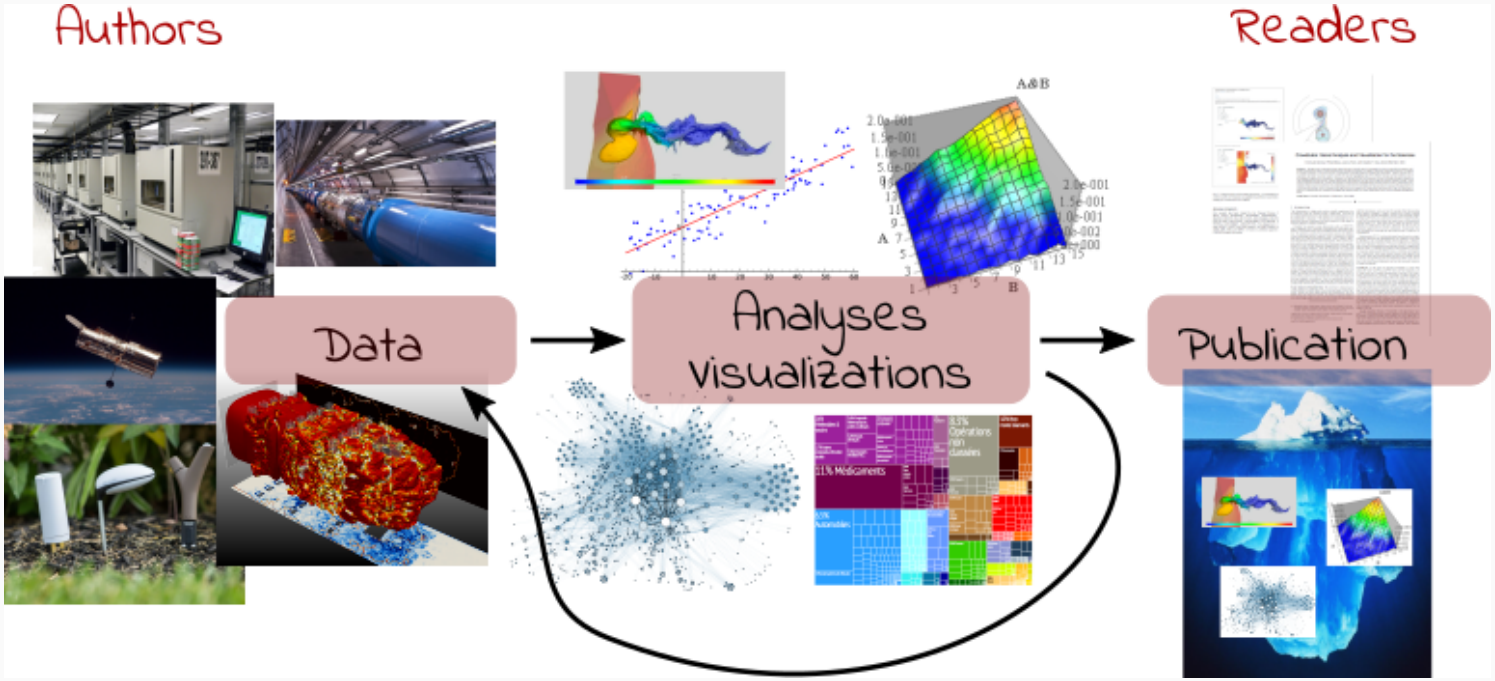


Reproducible Research = Bridging the Gap by working Transparently

Reproducible Research Practices

"Reproducible Research": First Appearance

Claerbout & Karrenbach, meeting of the Society of Exploration Geophysics, 1992

Electronic Documents Give Reproducible Research a New Meaning **RE1.3**

Jon F. Claerbout and Martin Karrenbach, Stanford Univ.

SUMMARY

A revolution in education and technology transfer follows from the marriage of word processing and software command scripts. In this marriage an author attaches to every figure caption a pushbutton or a name tag usable to recalculate the figure from all its data, parameters, and programs. This provid[illegible] of reproducibility in compute[illegible]

In 1990, we set this sequence of goals:

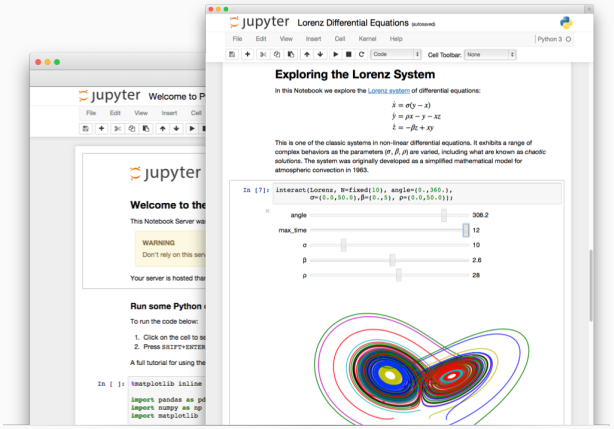
- Learn how to merge a publication with its underlying computational analysis.
- Teach researchers how to prepare a document in a form where they themselves can reproduce their own research results a year or more later by "pressing a single button".
- Learn how to leave finished work in a condition where coworkers can reproduce the calculation including the final illustration by pressing a button in its caption.
- Prepare a complete copy of our local software environment so that graduating students can take their work away with them to other sites, press a button, and reproduce their Stanford work.
- Merge electronic documents written by multiple authors (SEP reports).
- make incremental improvements in electronic-document software
- seek partners for broadening standards (and making incremental improvements).

Our basic goal is reproducible research. The electronic document is our means to this end. In principle, reproducibility in research can be achieved without electronic documents and that is how we started. Our first nonelectronic reproducible document was a textbook in which the paper document contained the name of a program script in every figure caption. The program scripts were organized by book chapter and section so they could be correlated to an accompanying magnetic tape dump of the file system. The magnetic tape also contained all the necessary data to feed the program script.

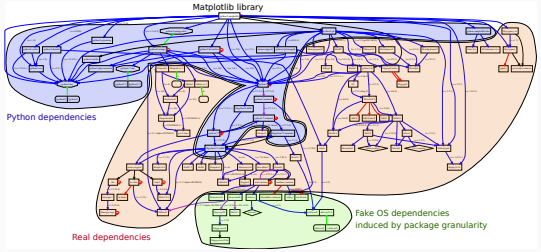
Now that we have begun using CD-ROM publication, we can go much further. Every figure caption contains a pushbutton that jumps to the appropriate science directory (folder) and initiates a figure rebuild command and then displays the figure, possibly as a movie or interactive program. We normally display seismic images of the earth's interior. but to reach wider audiences, Figure 1 shows a satellite weather picture which the pushbutton will animate as seen on commerical television. We include all our plot software as well as freely available software from many sources, including compilers and the LaTeX word processing system. Naturally

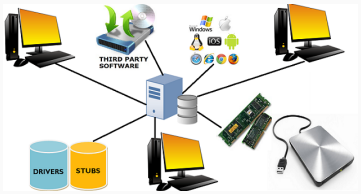
Existing Tools, Emerging Standards

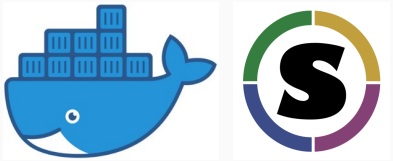
Notebooks and workflows



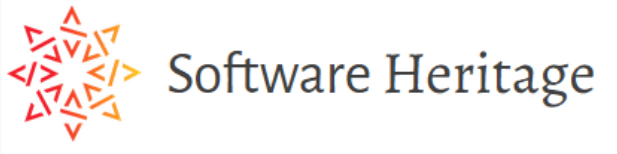
Software environments







Sharing platforms



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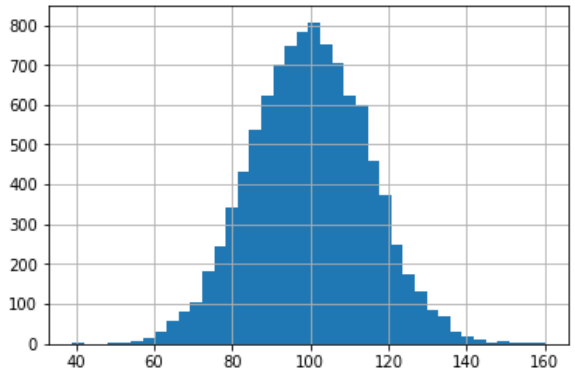
On peut inclure des formules mathématiques comme $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ et des *dessins qui n'ont rien à voir* avec π (si ce n'est une constante de normalisation... ☺).



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

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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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In [2]:

Hide Prompts Hide Code Hide Outputs

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Out[2]: 3.1437198694098765

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```

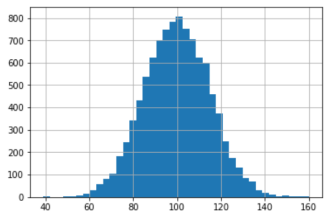
In [3]:

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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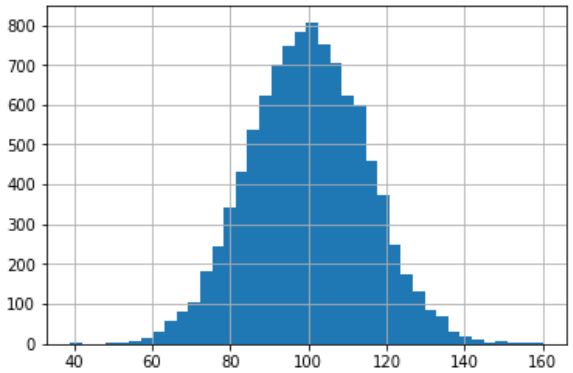

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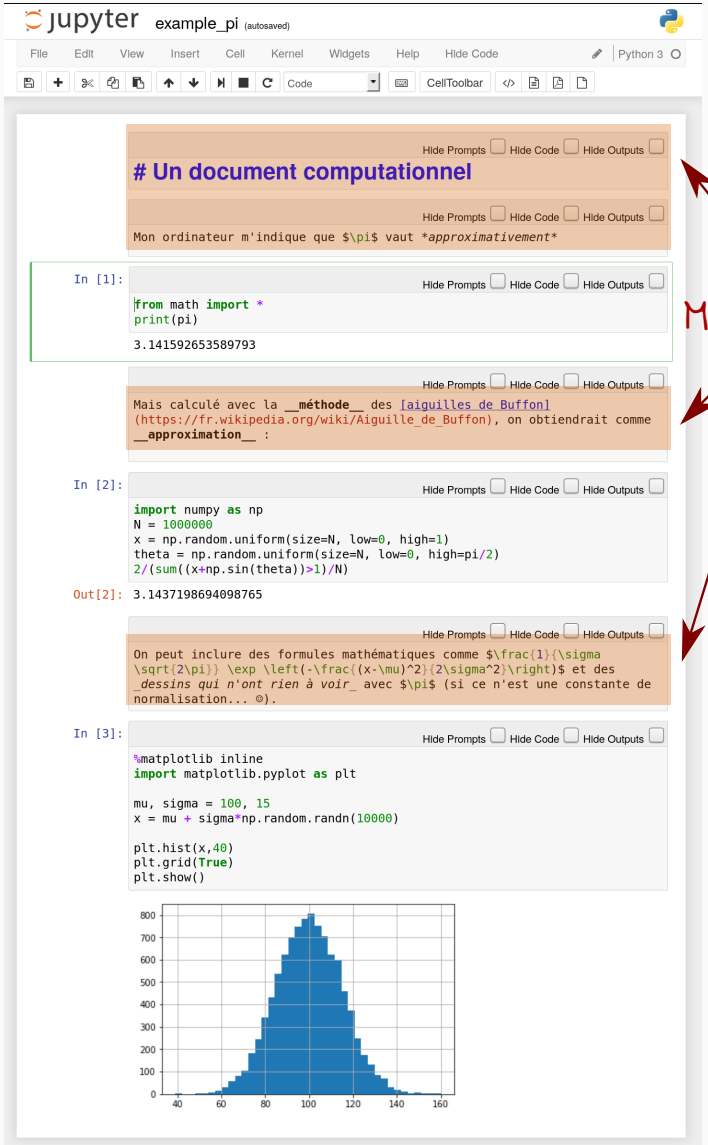

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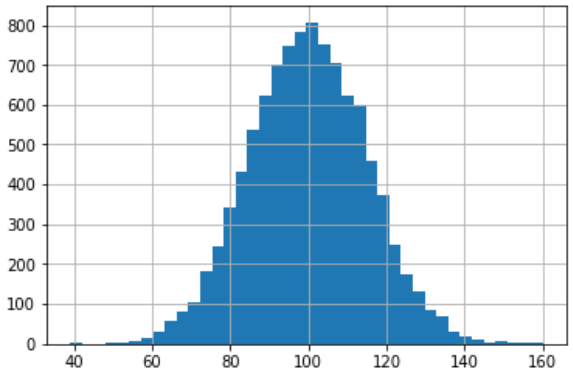

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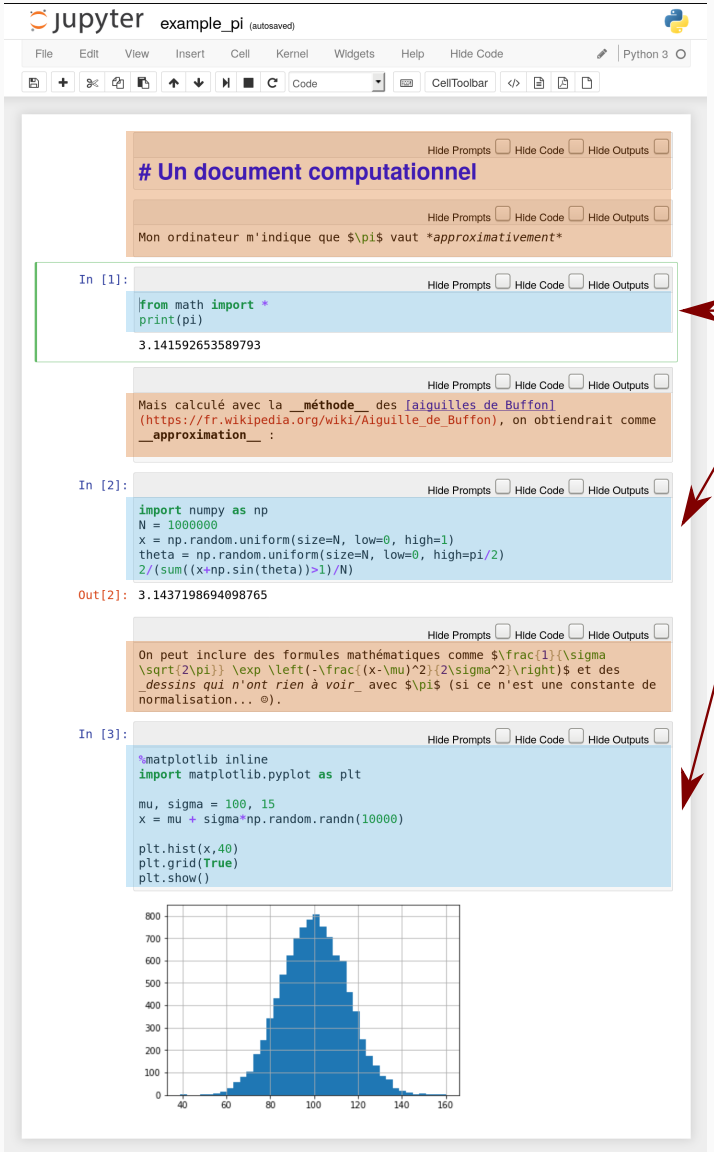


Code

Document final

Un document computationnel

Mon ordinateur m'indique que π vaut *approximativement*

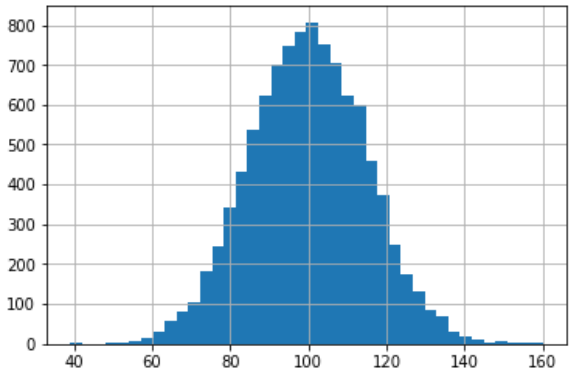
```
3.141592653589793
```

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)
```

```
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

Résultats

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
```

Hide Prompts Hide Code Hide Outputs

```
Mon ordinateur m'indique que $\pi$ vaut *approximativement*
```

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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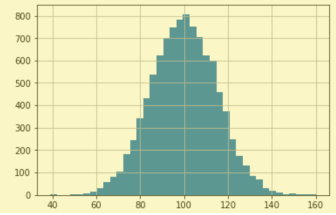
In [3]:

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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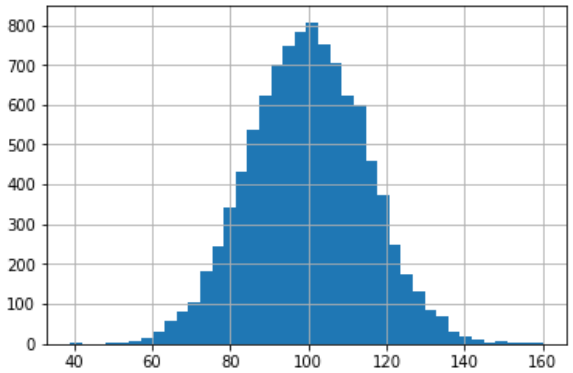

Tool 1: Computational Notebooks/Litterate Programming

Document initial dans son environnement

jupyter example_pi (autosaved)

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

Code CellToolbar

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# Un document computationnel
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Hide Prompts Hide Code Hide Outputs

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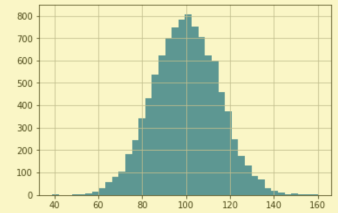

Export

Document final

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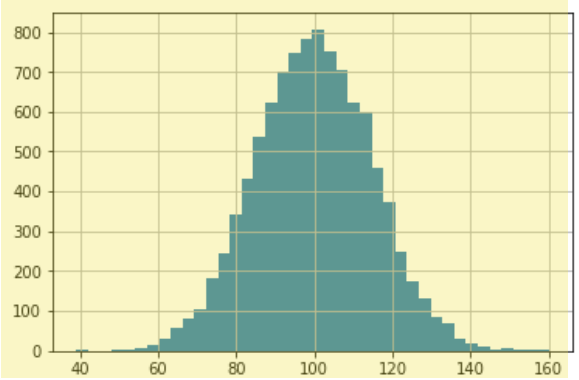

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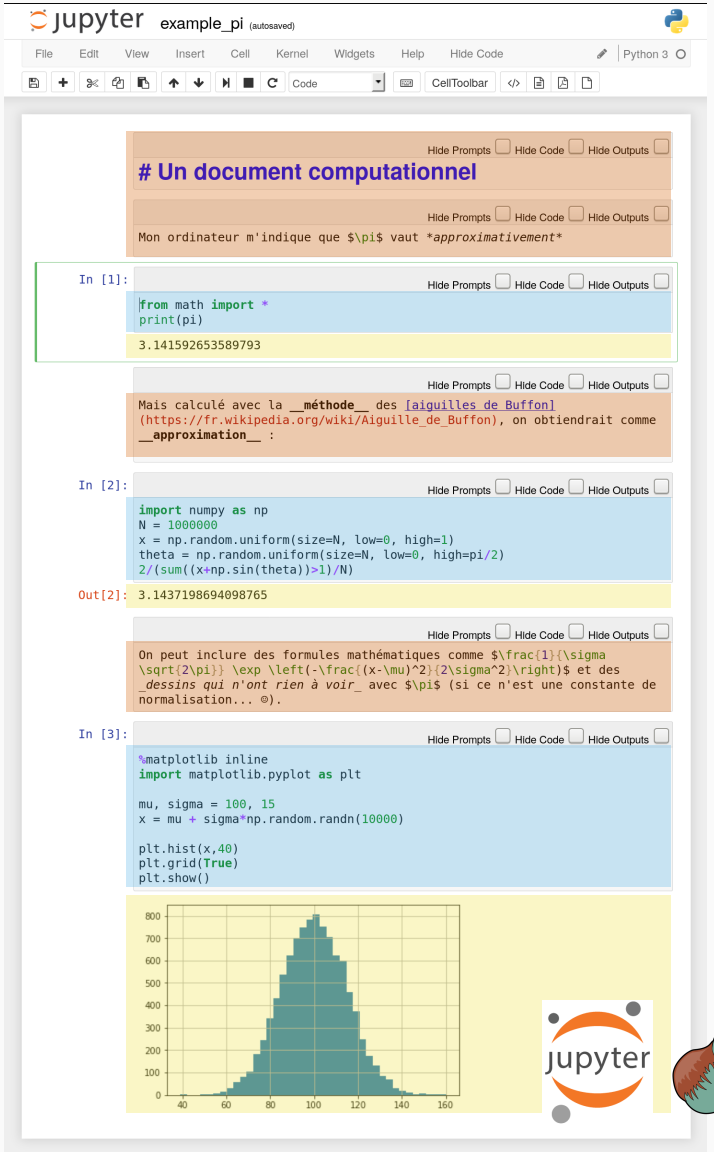

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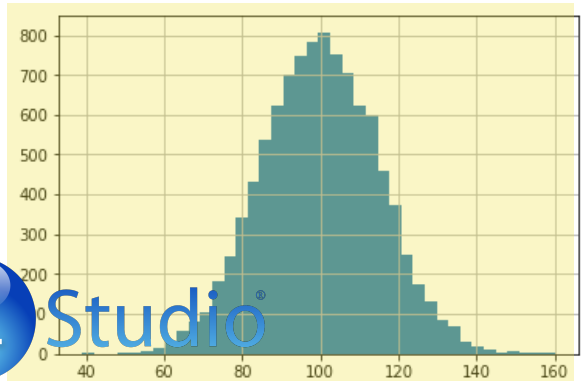

https://juyterhub.u-ga.fr/

Tool 2: Fighting Software Environments Nightmare

What is hiding behind a simple

```
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)
```

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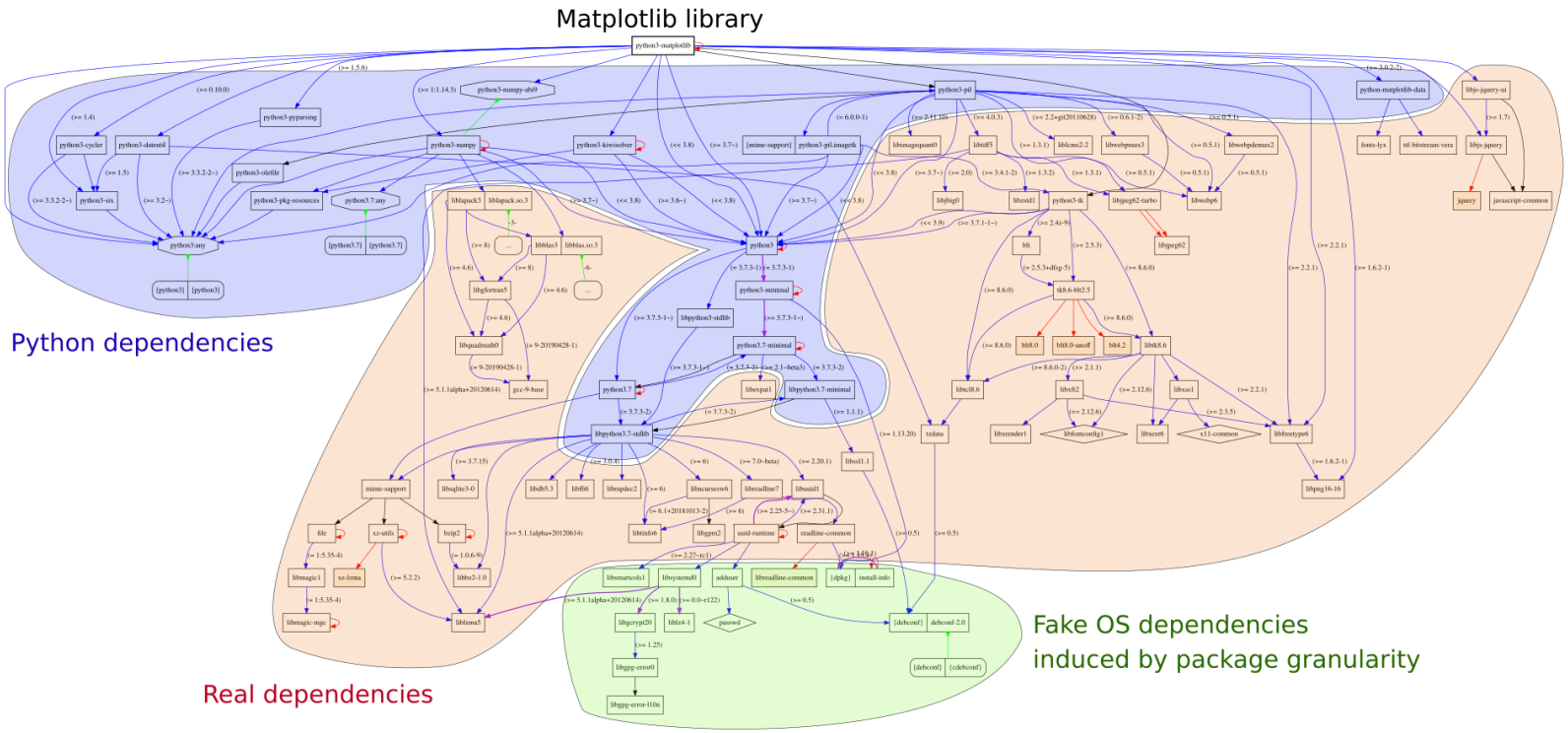

Tool 2: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

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

```
3
3.3333333333333335
```

Tool 2: Fighting Software Environments Nightmare

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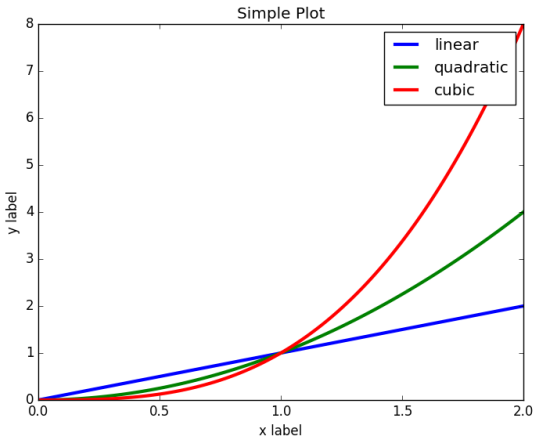

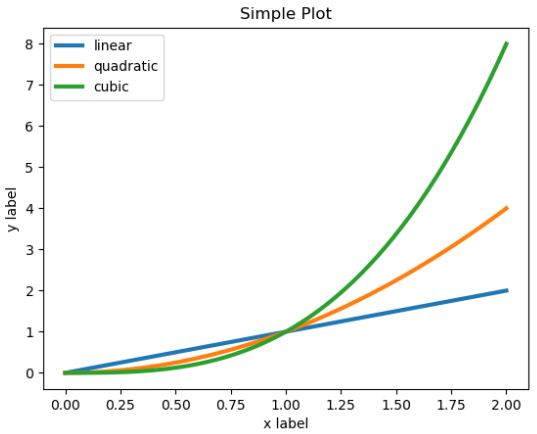

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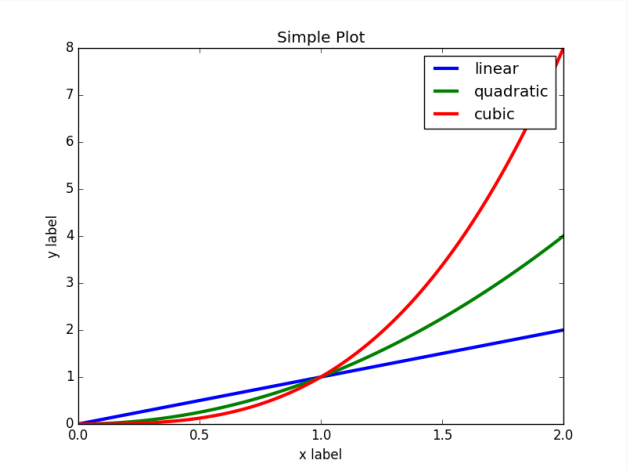

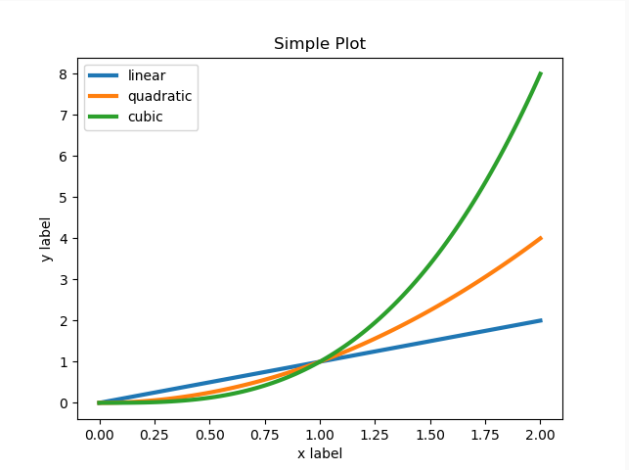

Cortical Thickness Measurements (PLOS ONE, June 2012) *FreeSurfer: differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

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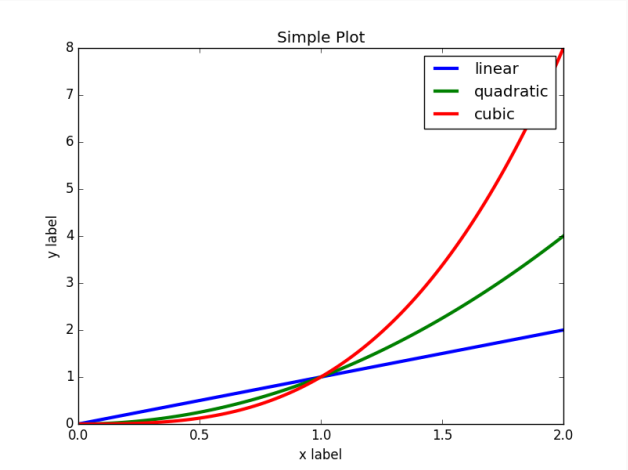

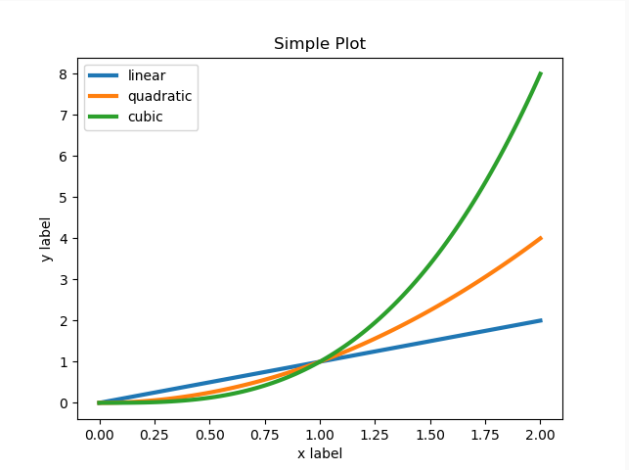

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ReproZip

Guix

Tool 3: Fighting Information Loss with Archives

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Article archives arXiv.org HAL archives-ouvertes.fr

Data archives figshare zenodo

Software Archive Software Heritage

INTERNET ARCHIVE

or = awesome collaborations (≠ archive)

What Will it Take ?

Changing Research Practices

Soft. Engineering, Statistics, and Reproducible Research in the curricula

Manifesto: *"I solemnly pledge"* (WSSSPE, Lorena Barba, FAIR)

1. I will teach my graduate students about reproducibility
2. All our research code (and writing) is under version control
3. We will always carry out verification and validation
4. We will share data, plotting script & figure under CC-BY
5. We will upload the preprint to arXiv at the time of submission of a paper
6. We will release code at the time of submission of a paper
7. We will add a "Reproducibility" declaration at the end of each paper
8. I will keep an up-to-date web presence

Changing Publishing Practices

Artifact evaluation and ACM badges

Major conferences

- Supercomputing: Artifact Description (AD) mandatory, Artifact Evaluation (AE) still optional, Double blind vs. RR
- NeurIPS, ICLR: open reviews, reproducibility challenge

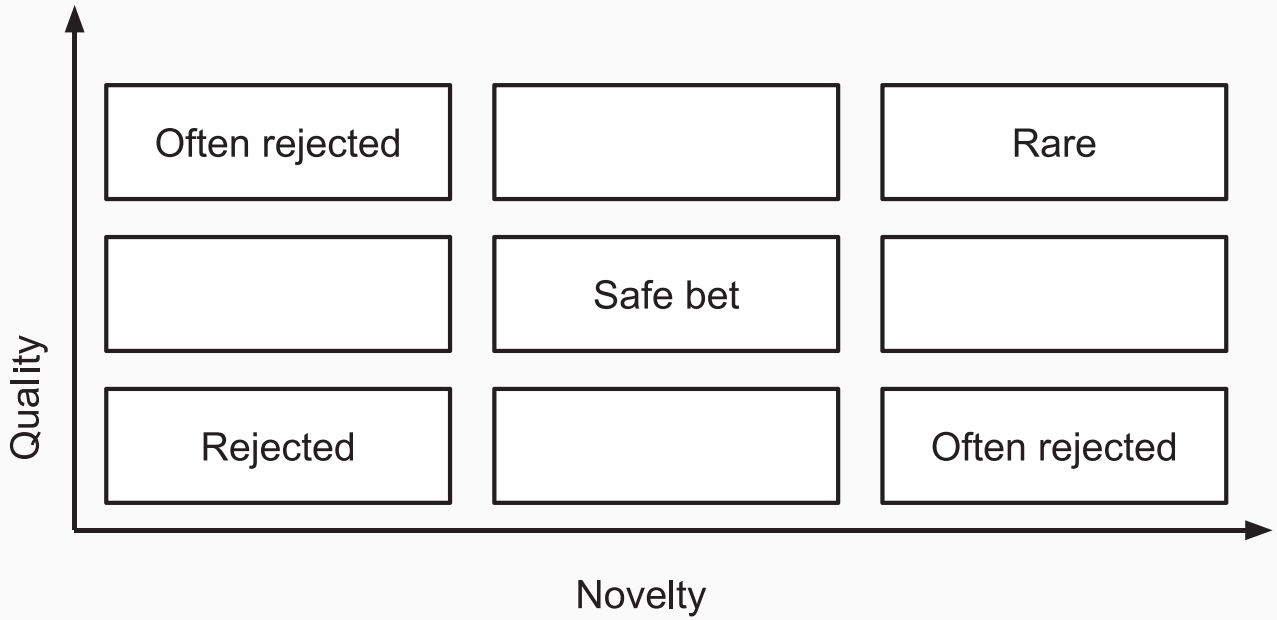
Joelle Pineau @ NeurIPS'18

- ACM SIGMOD 2015-2019, Most Reproducible Paper Award...

Mentalitie are evolving people care, make stuff available, errors are found and fixed

Changing Academic Practices (~~Publish or Perish~~)

- Goodhart's Law: Are Academic Metrics Being Gamed?, M. Fire 2019
  - AI: over 1,000 ranked journals (×10 in 15 years)
  - Shorter papers with increasing self references
  - More and more papers without any citation
  - Sharp increase in the number of new authors publishing at a much faster rate given their career age
- The Truth, The Whole Truth, and Nothing But the Truth: A Pragmatic, Guide to Assessing Empirical Evaluations, *TOPLAS* 2016



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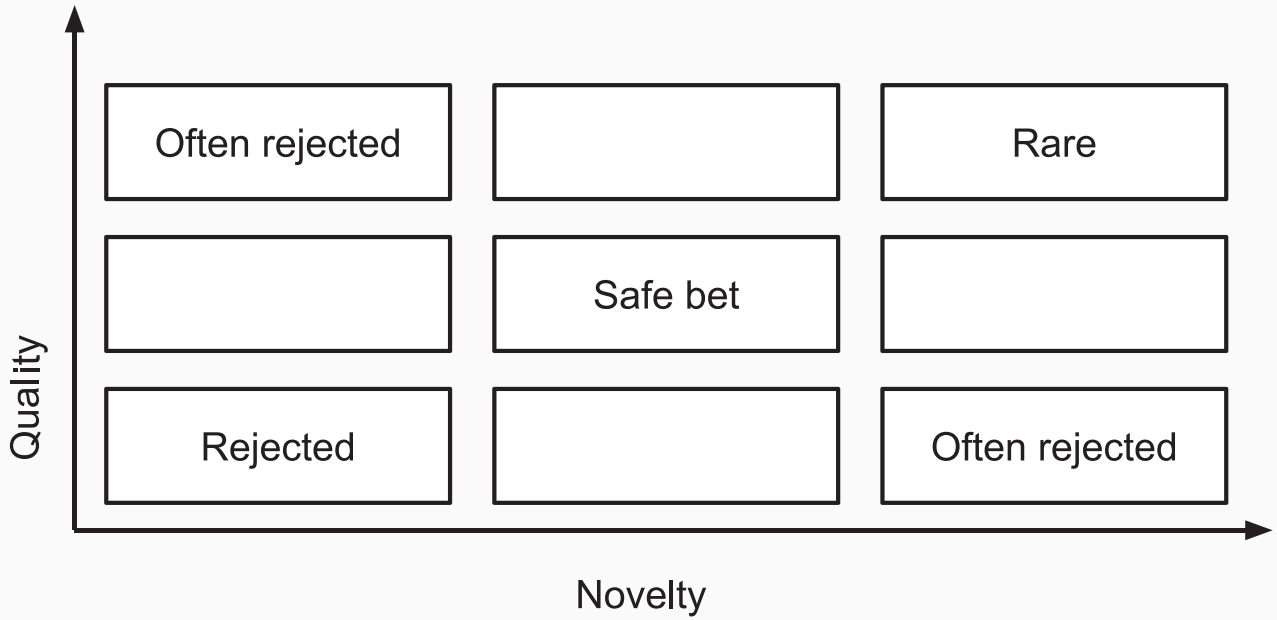


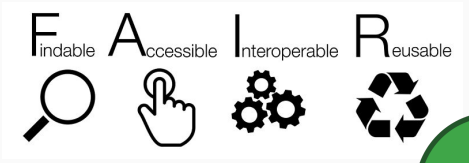
What about Open Science ?

Plan National pour la Science Ouverte (BSN ⇝ CoSO)

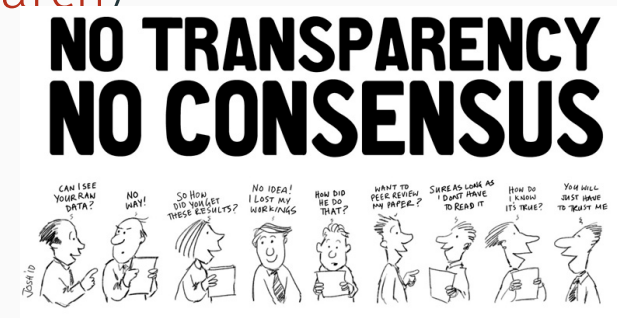
- CNRS, Inria, INRAE, ...
- Many flavors: *Citizen Science*

Main pillars:

1. Open access
2. Open data



3. Open source
   - *Open hardware*
4. **Open methodology** (Reproducible Research)
   - *Open-notebook science*
   - *Open science infrastructures*



5. Open peer review
6. Open educational resources

Resources and Acknowledgments

A non-technical introduction to reproducibility issues (in French)

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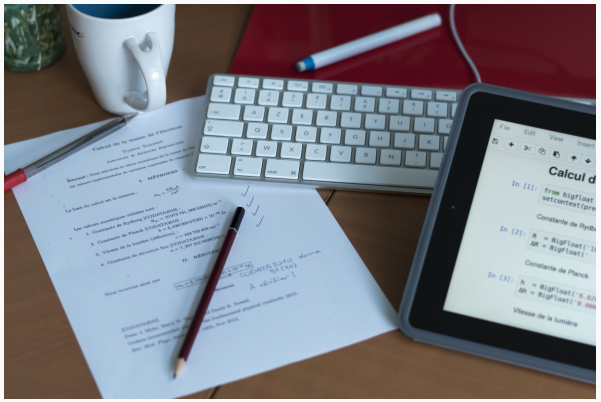
MOOC Reproducible Research: Methodological principles for a transparent science, Learning Lab Inria

- Konrad Hinsen, Christophe Pouzat
- 3rd Edition: March 2020 – March 2022
- MOOC RR "Advanced" planned for 2021
  - Software environment control
  - Scientific workflow
  - Managing data