

# REPRODUCIBILITY CRISIS AND OPEN SCIENCE

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Arnaud Legrand



Sciences de l'information géographique reproductibles  
June 2021



# PUBLIC EVIDENCE FOR A LACK OF REPRODUCIBILITY

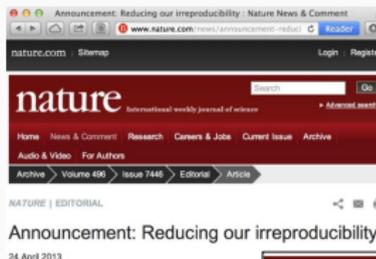
- J.P. Ioannidis. *Why Most Published Research Findings Are False* PLoS Med. 2005.
- *Lies, Damned Lies, and Medical Science*, The Atlantic. Nov, 2010
- *Reproducibility: A tragedy of errors*, Nature, Feb 2016.
- Steen RG, *Retractions in the scientific literature: is the incidence of research fraud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



LOCAL U.S. WORLD BUSINESS SPORTS ENTERTAINMENT HEALTH STYLE TRAVEL

## Science has lost its way, at a big cost to humanity

Researchers are rewarded for splashy findings, not for double-checking accuracy. So many scientists looking for cures to diseases have been building on ideas that aren't even true.



By Jef Axt | January 28, 2014

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  $\approx$  \$19 million from NIH
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**Diederik Stapel** Professor, Social Psychology, Univ. Tilburg, 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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58 retracted publications

**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

*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!*

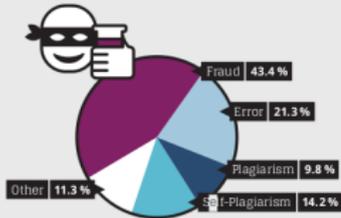
# A CREDIBILITY CRISIS?

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

## The Battle against Scientific Fraud in the CNRS International Magazine

### Biomedical fraud in figures

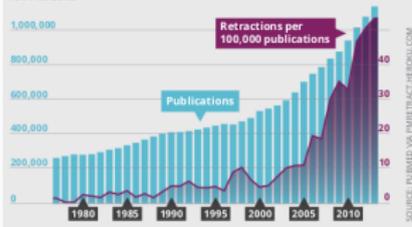
Cause of retraction 1977 to 2012



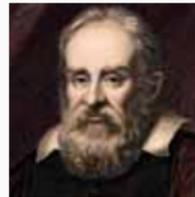
SOURCE: FANG ET AL. (2013) PNAS

Number of publications and retractions

1977 to 2013



SOURCE: PUBMED VS PUBTRACT-MEDICALL.COM



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

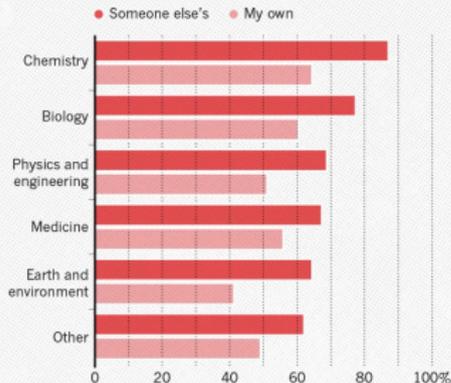
Scientific misconduct is obviously wrong but it's **not new!**

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

# A REPRODUCIBILITY CRISIS?

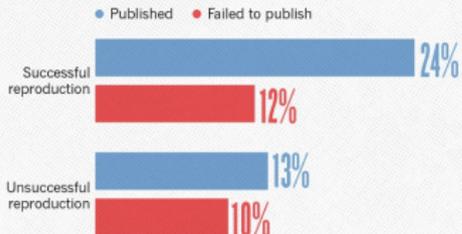
## HAVE YOU FAILED TO REPRODUCE AN EXPERIMENT?

Most scientists have experienced failure to reproduce results.



## HAVE YOU EVER TRIED TO PUBLISH A REPRODUCTION ATTEMPT?

Although only a small proportion of respondents tried to publish replication attempts, many had their papers accepted.



Number of respondents from each discipline:  
Biology 703, Chemistry 106, Earth and environmental 95,  
Medicine 203, Physics and engineering 236, Other 233

1,500 scientists lift the lid on reproducibility,

Nature, May 2016

## Social causes

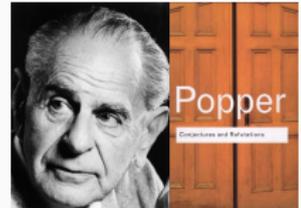
- Fraud, conflict of interest (pharmaceutic, ...)
- **No incentive** to reproduce/check our own work (afap), nor the work of others (big results!), nor to allow others to check (competition)
- Peer review does not scale: 1+ million articles per year!

## 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

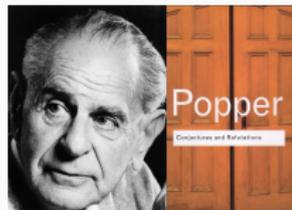
1934: Karl Popper puts the notions of **falsifiability** and **crucial experiment** as the **hallmark of science**

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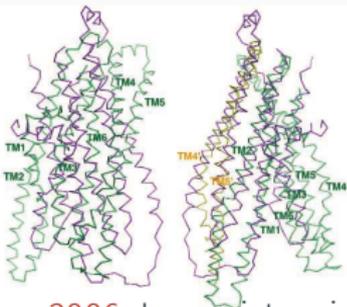
But, **scientific practices have greatly evolved**, in particular since we rely on **computers**



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

– Ben Marwick, The conversation, 2015

# HOW COMPUTERS BROKE SCIENCE



Geoffrey Chang (Scripps, UCSD) works on crystallography and studies the structure of cell membrane proteins.

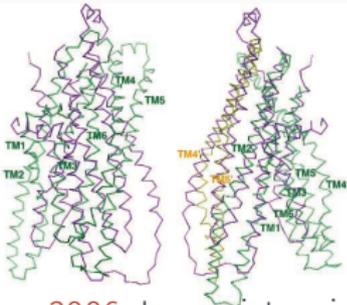
He specialized in structures of **multidrug resistant transporter proteins in bacteria**: MsbA de Escheria Choli (Science, 2001), Vibrio cholera (Mol. Biology, 2003), Salmonella typhimurium (Science, 2005)

2006: Inconsistencies reveal **a programming mistake**

*A homemade data-analysis program had flipped two columns of data, inverting the electron-density map from which his team had derived the protein structure.*

5 retracts that motivate **improved software engineering practices** in comp. biology

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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*

Authors



Data

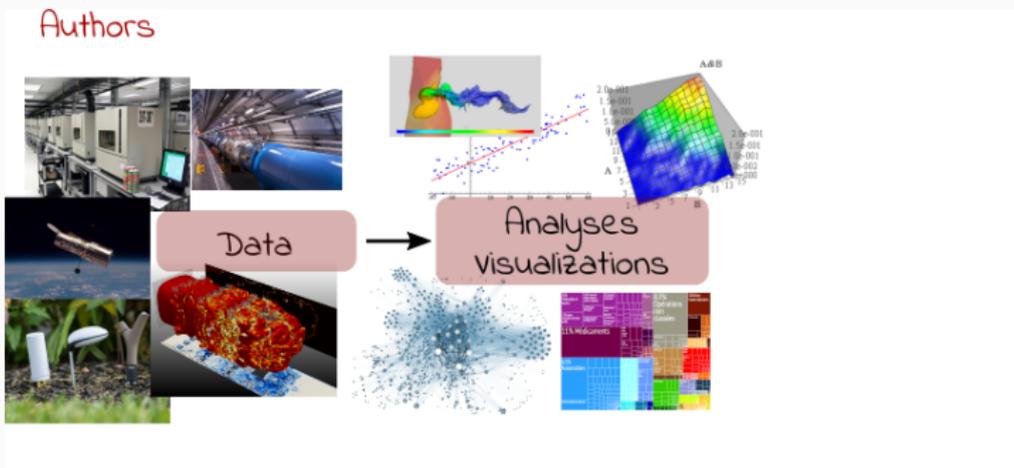
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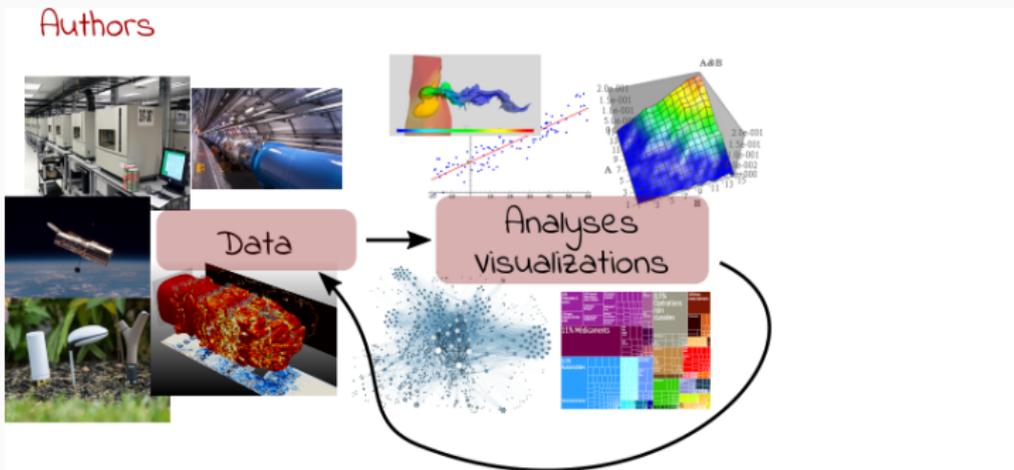
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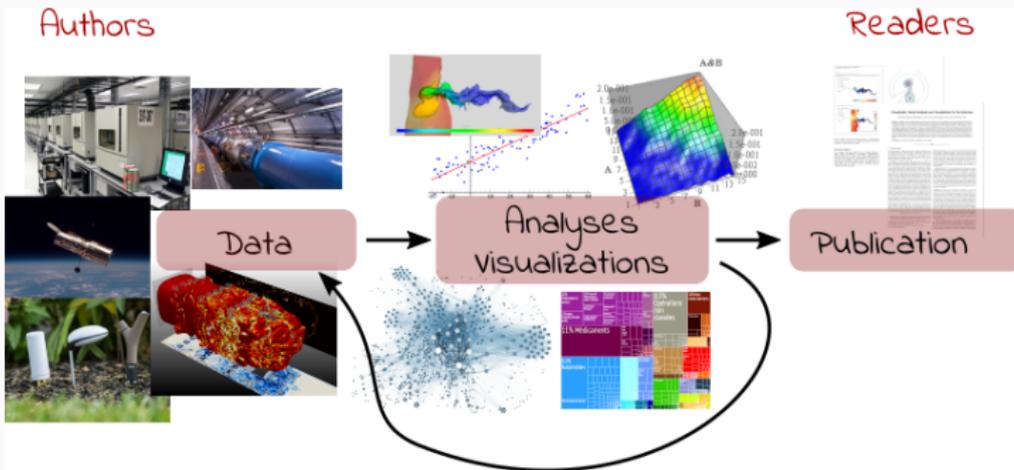
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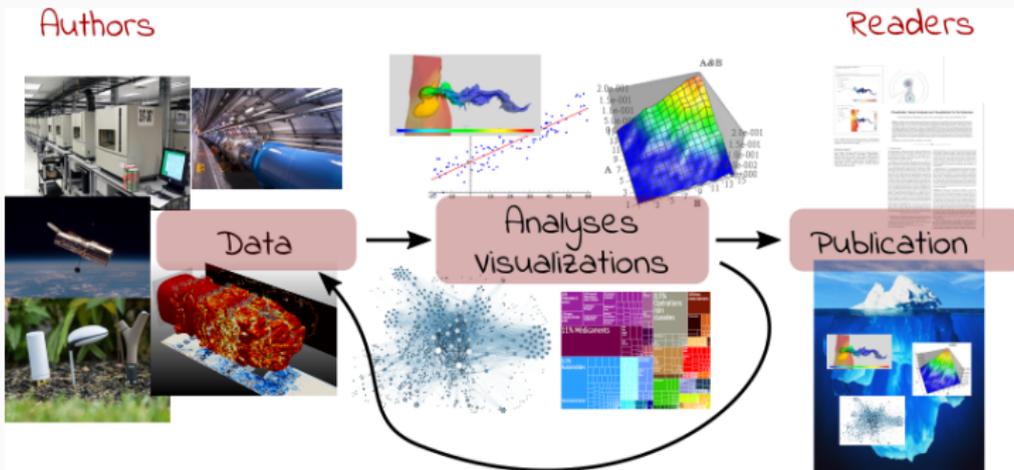
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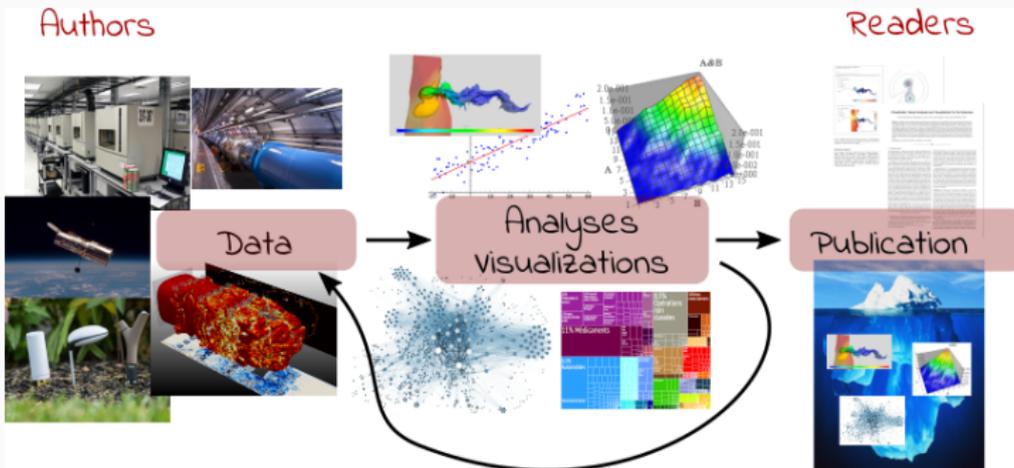
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Reproducible Research = Bridging the Gap by working Transparently

# REPRODUCIBLE RESEARCH PRACTICES

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# "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 provides a new level of reproducibility in computer graphics.

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 commercial television. We include all our plot software as well as freely available software from many sources, including compilers and the  $\text{\LaTeX}$  word processing system. Naturally we must include licensed software, but with the exception

# REPRODUCIBILITY, REPLICABILITY, ROBUSTNESS, GENERALIZATION

## REPRODUCIBLE



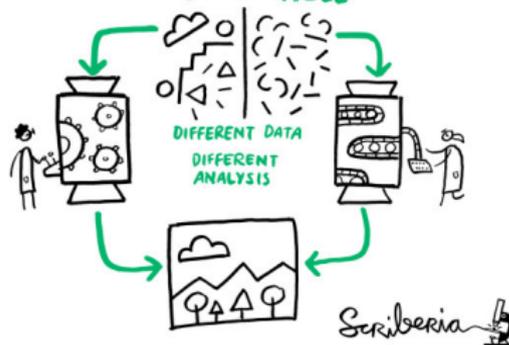
## REPLICABLE



## ROBUST



## GENERALISABLE



Scriberia 

# REPRODUCIBILITY (GLOSSARY MAY VARY)

Many **definitions** (*replicability, repeatability, reproducibility*), sometimes conflicting  
(*new data, same person, independent researcher*)

<b>experimental</b> reproducibility	similar input (data) + similar experimental protocol	→	<b>similar results</b> <sup>1</sup>
<b>statistical</b> reproducibility	different input (data) + same analysis	→	<b>same conclusions</b> <sup>2</sup>
<b>computational</b> reproducibility	similar input (data) + same code/software + same software environment	→	<b>exact same results</b> <sup>3</sup>

Reproducible Research = A way of doing science so that scientific experiments, discoveries, results, etc. can be easily reproduced (done again), to be confirmed, or to be built on for the next study.

– Courtesy G. Durriif, 2021

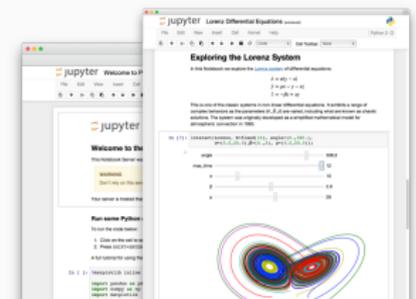
<sup>1</sup>Up-to measurement variability and precision

<sup>2</sup>Independently from (random) sampling variability (fight bias)

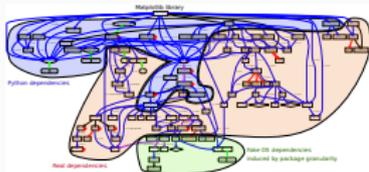
<sup>3</sup>Bitwise

# EXISTING TOOLS, EMERGING STANDARDS

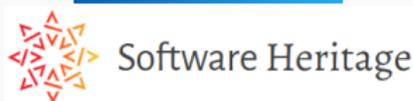
## Notebooks and workflows



## Software environments



## Sharing platforms



GOOD PRACTICE #1

TAKING NOTES AND DOCUMENTING

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# FRUSTRATION AS AN AUTHOR/REVIEWER



## Author

- I thought I used the same parameters but I'm getting different results!
- The new student wants to compare with the method I proposed last year
- My advisor asked me whether I took care of setting this or this but I can't remember
- The damned fourth reviewer asked for a major revision and wants me to change Figure 3. Which code and which data set did I use?
- It worked yesterday! 6 months later: Why did I do that?

## Reviewer

- As usual, there is no confidence interval, I wonder about the variability and whether the difference is significant or not
- That can't be true, I'm sure they removed some points
- Why is this graph in logscale? How would it look like otherwise? I'm not even sure of what this value means. If only I could access the generation script

## Un document computationnel

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

3.141592653589793

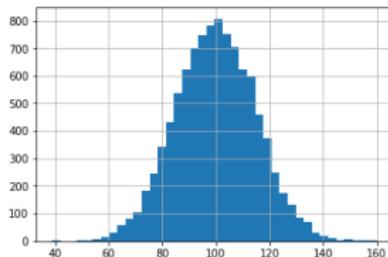
Mais calculé avec la **méthode** des [aiguilles de Buffon](#), on obtiendrait comme **approximation** :

```
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  $\pi$  (si ce n'est une constante de normalisation... ☹).



# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Document initial dans son environnement



The screenshot shows a Jupyter Notebook titled "example\_pi" with a Python 3 kernel. The notebook content is as follows:

```
# Un document computationnel
```

Mon ordinateur m'indique que  $\pi$  vaut "approximativement"

```
In [1]:
```

```
from math import *
print(pi)
3.141592653589793
```

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

```
In [2]:
```

```
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```

```
Out[2]:
```

```
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```

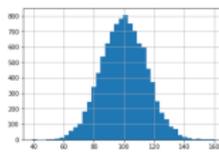
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```
In [3]:
```

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

mu, sigma = 100, 35
x = mu + sigma*np.random.randn(10000)

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



## Document final

### Un document computationnel

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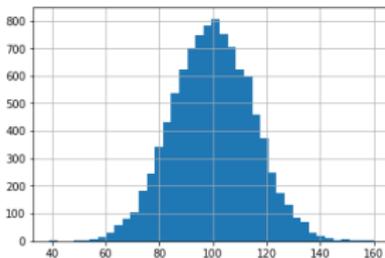
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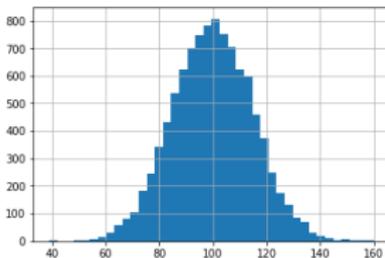
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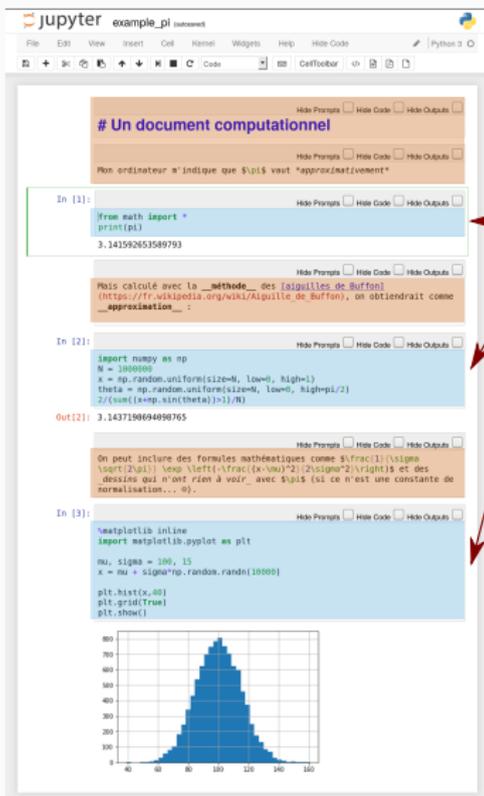
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- Cell 1: A title cell containing "# Un document computationnel".
- Cell 2: A text cell containing "Mon ordinateur m'indique que  $\pi$  vaut *approximativement*".
- Cell 3: A code cell with `from math import *` and `print(pi)`, outputting `3.141592653589793`.
- Cell 4: A text cell containing "Mais calculé avec la méthode des aiguilles de Buffon ([https://fr.wikipedia.org/wiki/Aiguille\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Aiguille_de_Buffon)), on obtiendrait comme approximation :".
- Cell 5: A code cell with `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)`, and `2/(sum((x+np.sin(theta))>1)/N)`, outputting `3.1437198694098765`.
- Cell 6: A text cell containing "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  $\pi$  (si ce n'est une constante de normalisation... ☺)".
- Cell 7: A code cell with `import matplotlib.pyplot as plt`, `mu, sigma = 100, 15`, `x = mu + sigma*np.random.randn(10000)`, `plt.hist(x, 40)`, `plt.grid(True)`, and `plt.show()`, followed by a histogram plot.

Code

## Document final

### Un document computationnel

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

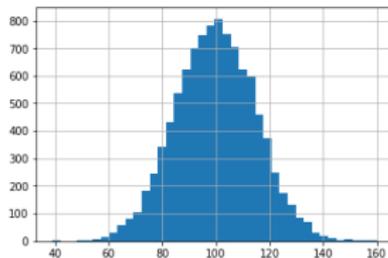
3.141592653589793

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  $\pi$  (si ce n'est une constante de normalisation... ☺).



# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Document initial dans son environnement

The screenshot shows a Jupyter Notebook interface with the following content:

- Cell 1:** A title cell containing "# Un document computationnel".
- Cell 2:** A text cell containing "Mon ordinateur m'indique que  $\pi$  vaut *approximativement*".
- Cell 3:** A code cell with the following code:

```
from math import *\nprint(pi)
```

The output is "3.141592653589793".
- Cell 4:** A text cell containing "Mais calculé avec la *méthode* des *aiguilles de Buffon* ([https://fr.wikipedia.org/wiki/Aiguille\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Aiguille_de_Buffon)), on obtiendrait comme *approximation* :".
- Cell 5:** A code cell with the following code:

```
import numpy as np\nN = 1000000\nx = np.random.uniform(size=N, low=0, high=1)\ntheta = np.random.uniform(size=N, low=0, high=pi/2)\n2/(sum((x+np.sin(theta))>1)/N)
```

The output is "3.1437198694098765".
- Cell 6:** A text cell containing "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  $\pi$  (si ce n'est une constante de normalisation... ☺)".
- Cell 7:** A code cell with the following code:

```
import matplotlib\nimport matplotlib.pyplot as plt\nmu, sigma = 100, 15\nx = mu + sigma*np.random.randn(10000)\nplt.hist(x, 40)\nplt.grid(True)\nplt.show()
```

The output is a histogram showing a normal distribution centered at 100.

Résultats

## Document final

### Un document computationnel

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

3.141592653589793

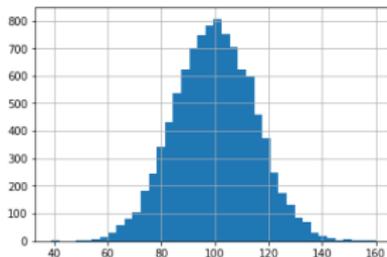
Mais calculé avec la *méthode* des *aiguilles de Buffon*, on obtiendrait comme *approximation* :

```
import numpy as np\nN = 1000000\nx = np.random.uniform(size=N, low=0, high=1)\ntheta = np.random.uniform(size=N, low=0, high=pi/2)\n2/(sum((x+np.sin(theta))>1)/N)
```

3.1437198694098765

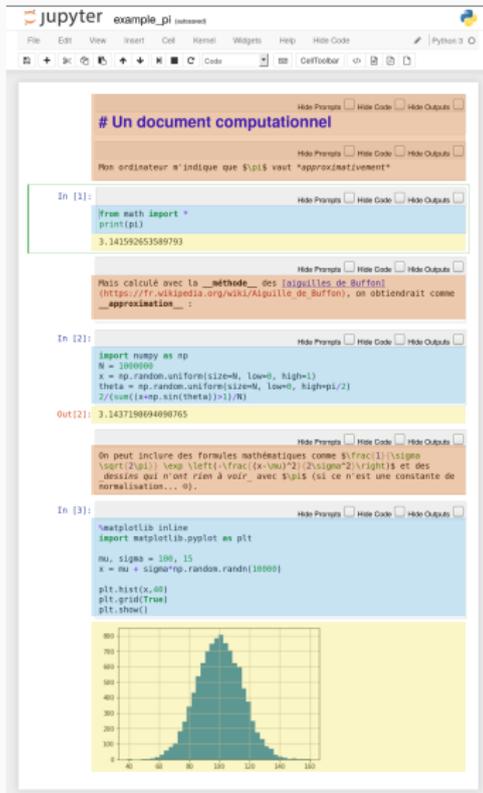
On peut inclure des formules mathématiques comme  $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$  et

des *dessins qui n'ont rien à voir* avec  $\pi$  (si ce n'est une constante de normalisation... ☺).



# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Document initial dans son environnement



The screenshot shows a Jupyter Notebook interface with the following content:

- Header: # Un document computationnel
- Text: Mon ordinateur m'indique que  $\pi$  vaut *approximativement*
- Code cell (In [1]):

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

Output: 3.141592653589793
- Text: Mais calculé avec la *méthode* des *aiguilles de Buffon* ([https://fr.wikipedia.org/wiki/Aiguille\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Aiguille_de_Buffon)), on obtiendrait comme *approximation* :
- Code cell (In [2]):

```
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)
Z/(sum((x+np.sin(theta))>1)/N)
```

Output: 3.1437198694098765
- Text: 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  $\pi$  (si ce n'est une constante de normalisation... ☺).
- Code cell (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)
plt.show()
```
- Figure: A histogram showing a normal distribution centered at 100, with a peak frequency of approximately 800.

Export

## Document final

### Un document computationnel

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

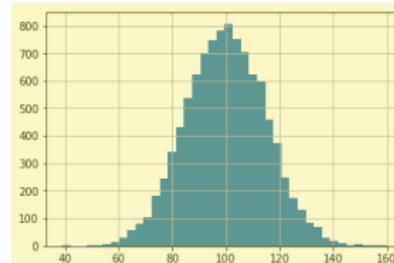
3.141592653589793

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)
Z/(sum((x+np.sin(theta))>1)/N)
```

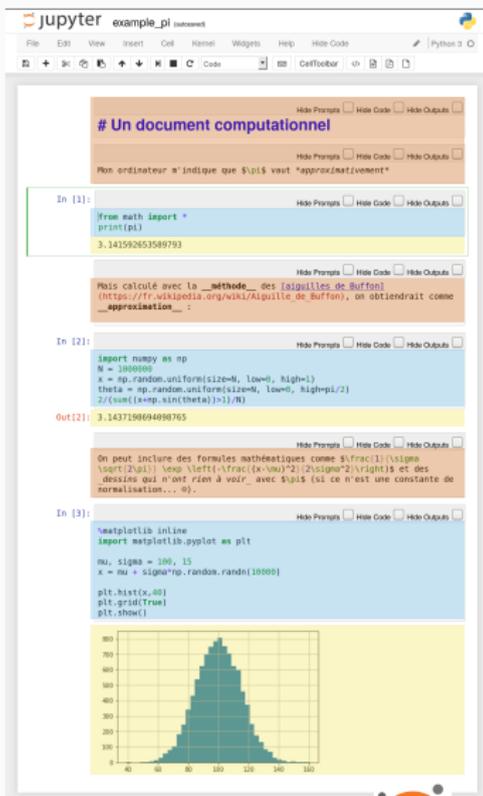
3.1437198694098765

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  $\pi$  (si ce n'est une constante de normalisation... ☺).



# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Document initial dans son environnement



The screenshot shows a Jupyter Notebook interface with the following content:

```
# Un document computationnel
```

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

```
In [1]: from math import *\nprint(pi)\n3.141592653589793
```

Mais calculé avec la méthode des aiguilles de Buffon ([https://fr.wikipedia.org/wiki/Aiguille\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Aiguille_de_Buffon)), on obtiendrait comme approximation :

```
In [2]: import numpy as np\nN = 1000000\nx = np.random.uniform(size=N, low=0, high=1)\ntheta = np.random.uniform(size=N, low=0, high=pi/2)\n2/(sum((x+np.sin(theta))>1)/N)\nOut[2]: 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  $\pi$  (si ce n'est une constante de normalisation... ☺).

```
In [3]: %matplotlib inline\nimport matplotlib.pyplot as plt\nmu, sigma = 100, 15\nx = mu + sigma*np.random.randn(10000)\nplt.hist(x, 40)\nplt.grid(True)\nplt.show()
```



## Document final

### Un document computationnel

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

3.141592653589793

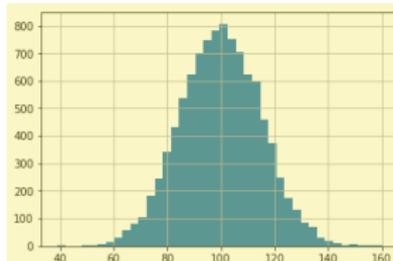
Mais calculé avec la méthode des aiguilles de Buffon, on obtiendrait comme approximation :

```
import numpy as np\nN = 1000000\nx = np.random.uniform(size=N, low=0, high=1)\ntheta = np.random.uniform(size=N, low=0, high=pi/2)\n2/(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  $\pi$  (si ce n'est une constante de normalisation... ☺).



Document your:

- **Hypotheses**: keep track of your ideas/line of thoughts
- **Experiments**: details on how and why an experiment was run, including failed or ambiguous attempts
- **Initial analysis or interpretation of these experiments**: was the outcome conform to the expectation or not? does it (in)validate the hypothesis? **why** did you do this or that ?
- **Organization**: keep track of things to do/fix/test/improve

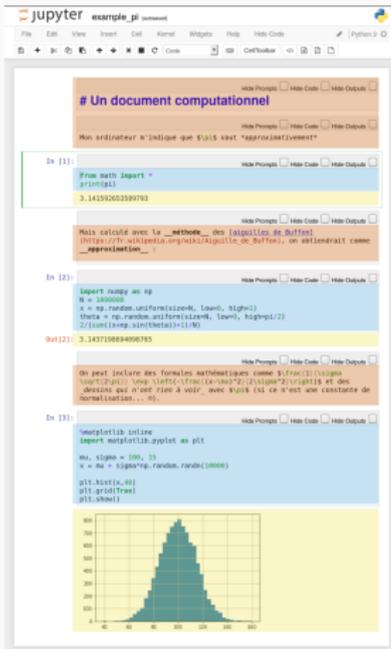
**Write for the future you**

I have a very intense usage of my journal and I can **demo this today**

- Experiment results are better **structured by dates** (add tags)
- Final rendering of results (figures, tables, article, presentation) should be reproducible
- Use plain text and lightweight markup languages (e.g.,  $\text{\LaTeX}$  or Markdown)

# TOOL 1 BIS: WORKFLOWS

Notebooks are no panacea and do not help developing clean code



The screenshot shows a Jupyter Notebook interface with the following content:

- Section Header:** `# Un document computationnel`
- Text:** `Mon ordinateur n'indique que j'ai écrit "approximativement"`
- Code Cell 1:**

```
In [1]: from math import *\n        print(pi)\n        3.141592653589793
```
- Text:** `Mais calculé avec la __methode__ des (ajoutées de Buffon)\n https://fr.wikipedia.org/wiki/Aiguille_de_Buffon, on obtiendrait comme\n __approximation__ :`
- Code Cell 2:**

```
In [2]: import numpy as np\n        N = 100000\n        x = np.random.uniform(size=N, low=0, high=1)\n        theta = np.random.uniform(size=N, low=0, high=np.pi/2)\n        Z = sum((np.sin(theta))**2)/N\n        Out[2]: 3.143710684006763
```
- Text:** `On peut inclure des formules mathématiques comme  $\frac{1}{\sqrt{2\pi}}$  dans\n sqrt(2*pi),  $\frac{1}{\sqrt{2\pi}}$  dans 1/sqrt(2*pi) et des\n dérivés qui sont plus à voir, avec tout (si ce n'est une constante de\n normalisation... etc).`
- Code Cell 3:**

```
In [3]: import matplotlib\n        import matplotlib.pyplot as plt\n        mu, sigma = 100, 25\n        x = mu + sigma*np.random.randn(10000)\n        plt.hist(x,40)\n        plt.grid(True)\n        plt.show()
```
- Figure:** A histogram showing a normal distribution of data points, centered around 100, with a grid overlaid.

# TOOL 1 BIS: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

The screenshot shows a Jupyter Notebook interface with the following content:

- Header:** jupyter analyse-syndrome-grippal Last Checkpoint: 20 minutes ago (sauveveit)
- Menu:** File Edit View Insert Cell Kernel Widgets Help Hide Code
- Toolbar:** +, -, Run, Refresh, Stop, Save, Undo, Redo, Home, End, Esc, Help/Show code, Export to HTML
- Section 101: Incidence du syndrome grippal**
  - Code cell: `import pandas as pd`
  - Text cell: "Les données de l'incidence de syndromes respiratoires (RS) de 1999 à 2010, l'année 2010 est la base de données pour l'année 2010. Les données de l'année 2010 ont été ajoutées à la base de données de l'année 2009 pour permettre de faire un suivi de l'année 2010. Les données de l'année 2010 ont été ajoutées à la base de données de l'année 2009 pour permettre de faire un suivi de l'année 2010." (Note: The text in the image is partially obscured and appears to be a placeholder or a very short summary of the data source.)
  - Table: "Base de données" (Table with 10 columns: year, country, population, influenza, pneumonia, influenza\_and\_pneumonia, influenza\_and\_pneumonia\_per\_1000, influenza\_and\_pneumonia\_per\_1000\_per\_year, influenza\_and\_pneumonia\_per\_1000\_per\_year\_per\_1000, influenza\_and\_pneumonia\_per\_1000\_per\_year\_per\_1000\_per\_year)
  - Code cell: `df = pd.read_csv('data/influenza_and_pneumonia.csv')`
  - Code cell: `df.head()`
- Section 102: Analyse des données**
  - Code cell: `df.groupby('year').sum()`
  - Table: "Summary of influenza and pneumonia incidence by year" (Table with 2 columns: year, sum)
- Section 103: Visualisation**
  - Code cell: `df.groupby('year').sum().plot()`
  - Figure: A bar chart showing the sum of influenza and pneumonia incidence by year from 1999 to 2010. The x-axis is labeled 'year' and the y-axis is labeled 'sum'. The bars show a general upward trend with some fluctuations.

# TOOL 1 BIS: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

The image displays a Jupyter Notebook interface with a workflow for analyzing influenza data. The notebook is titled "analyse-epidemie-grippe1" and is running on a JupyterLab environment. The workflow consists of several cells:

- Cell 1:** A text cell containing a title "Epidémie de syndrome grippal" and a description of the data source (World Health Organization).
- Cell 2:** A code cell that loads the data into a pandas DataFrame. The output is a large table with columns for "Year", "Country", "Cases", "Deaths", and "Recovery".
- Cell 3:** A code cell that filters the data for the year 2009 and the country "France". The output is a smaller table with columns for "Year", "Country", "Cases", "Deaths", and "Recovery".
- Cell 4:** A code cell that calculates the percentage of cases, deaths, and recovery for the filtered data. The output is a table with columns for "Year", "Country", "Cases", "Deaths", "Recovery", and "Percentage".
- Cell 5:** A code cell that creates a bar chart showing the percentage of cases, deaths, and recovery for the filtered data. The chart has a title "Epidémie de syndrome grippal" and a y-axis labeled "Percentage".
- Cell 6:** A code cell that creates a line chart showing the percentage of cases, deaths, and recovery for the filtered data. The chart has a title "Epidémie de syndrome grippal" and a y-axis labeled "Percentage".
- Cell 7:** A code cell that creates a scatter plot showing the percentage of cases, deaths, and recovery for the filtered data. The chart has a title "Epidémie de syndrome grippal" and a y-axis labeled "Percentage".
- Cell 8:** A code cell that creates a bar chart showing the percentage of cases, deaths, and recovery for the filtered data. The chart has a title "Epidémie de syndrome grippal" and a y-axis labeled "Percentage".
- Cell 9:** A code cell that creates a bar chart showing the percentage of cases, deaths, and recovery for the filtered data. The chart has a title "Epidémie de syndrome grippal" and a y-axis labeled "Percentage".

## Notebooks are no panacea and do not help developing clean code

The image displays a series of Jupyter Notebook cells illustrating a machine learning pipeline for color classification. The workflow is as follows:

- Estimating Color Names by Web Image Services:** A cell showing code to fetch image URLs and their corresponding color names from a web service.
- Chromaticity plane and chromaticity model results:** A plot showing the distribution of colors in the chromaticity plane, with a model fit overlaid.
- Model Training:** A cell showing the training of a model on the chromaticity plane data.
- Model Evaluation:** A cell showing the evaluation of the model's performance on a test set.
- Chromaticity plane and chromaticity model results (repeated):** A second plot showing the distribution of colors in the chromaticity plane, with a model fit overlaid.
- Prediction error vs. Training sample variance:** A scatter plot showing the relationship between training sample variance and prediction error.
- Challenge: truth vs. prediction:** A confusion matrix plot showing the relationship between true and predicted values.



## Workflows:

- Clearer high-level view
- Composition of codes and data movement made explicit
- Safer sharing, reusing, and execution
- Notebooks are a variant that is both impoverished and richer
- No simple/mature path from a notebook to a workflow

## Examples:

- Galaxy, Kepler, Taverna, Pegasus, Collective Knowledge, VisTrails
- Light-weight: dask, drake, swift, snakemake, ...
- Hybrids: SOS-notebook, ...

GOOD PRACTICE #2

CONTROLLING SOFTWARE ENVIRONMENT

---

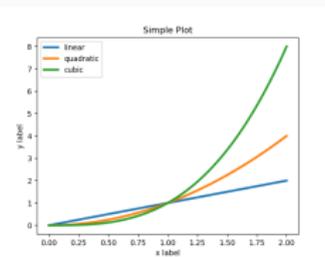
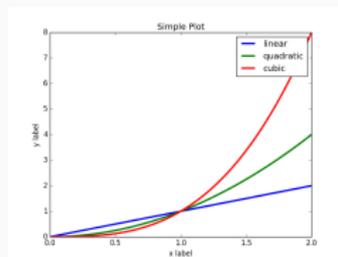
# ARGH... DAMNED COMPUTERS

- **Alice:** I got 3.123123                      **Bob:** I got segfault
- Damned! It used to work!!! Whenever I upgrade my computer, things break so I try to stay away from this 😞
- Anyway, I don't have the root password                      The what?...
- Whenever trying the code of my colleague, I had to install Foo but I broke everything and now neither his code nor mine works! 😞
- But hey! Here is my code, feel free to play with it! I'm doing open science 😊

Seriously ? How come all this is so painful ?

# BACKWARDS COMPATIBILITY

- Software environment evolution



- Software environment evolution
- Software evolution and OS heterogeneity

The Effects of FreeSurfer Version, Workstation Type, and Macintosh Operating System Version on Anatomical Volume and Cortical Thickness Measurements (PLOS ONE, 2012)

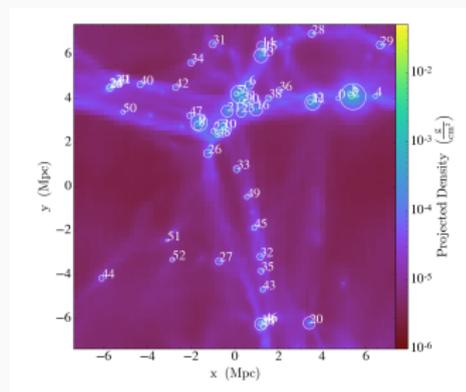
*Significant differences in volume and cortical thickness were revealed across FreeSurfer versions. In addition, less pronounced differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

# BACKWARDS COMPATIBILITY

- Software environment evolution
- Software evolution and OS heterogeneity
- Impact of the compiler

Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

Compiler	Optim.	Largest Halo Avg Mass.	Std. Err	Walltime
gcc@6.2.0	None	2.273E46	1.069E44	22h
gcc@6.2.0	Normal	2.266E46	1.218E44	10h
gcc@6.2.0	High	2.275E46	1.199E44	9h
intel@16.0.3	None	2.271E45	1.587E44	39h
intel@16.0.3	Normal	4.330(45)	1.248E44	7h
intel@16.0.3	High	2.268E46	1.414E44	6h
cce@8.5.5	Low	4.311(45)	1.353E44	16h
cce@8.5.5	Normal	2.271E46	1.261E44	6h
cce@8.5.5	High	2.272E46	1.341E44	5h

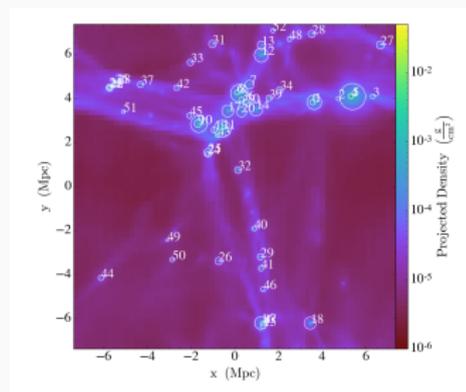


# BACKWARDS COMPATIBILITY

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gcc@6.2.0	High	2.275E46	1.199E44	9h
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intel@16.0.3	Normal	4.330(45)	1.248E44	7h
intel@16.0.3	High	2.268E46	1.414E44	6h
cce@8.5.5	Low	4.311(45)	1.353E44	16h
cce@8.5.5	Normal	2.271E46	1.261E44	6h
cce@8.5.5	High	2.272E46	1.341E44	5h

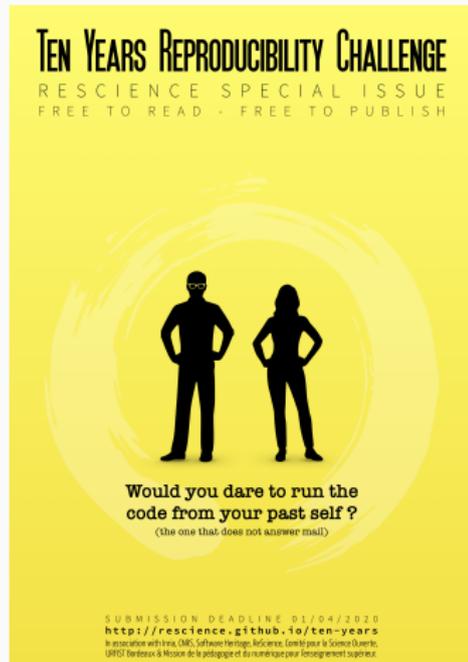


# BACKWARDS COMPATIBILITY

- Software environment evolution
- Software evolution and OS heterogeneity
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Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

Compiler	Optim.	Largest Halo Avg Mass.	Std. Err	Walltime
gcc@6.2.0	None	2.273E46	1.069E44	22h
gcc@6.2.0	Normal	2.266E46	1.218E44	10h
gcc@6.2.0	High	2.275E46	1.199E44	9h
intel@16.0.3	None	2.271E45	1.587E44	39h
intel@16.0.3	Normal	<b>4.330(45)</b>	1.248E44	7h
intel@16.0.3	High	2.268E46	1.414E44	6h
cce@8.5.5	Low	<b>4.311(45)</b>	1.353E44	16h
cce@8.5.5	Normal	2.271E46	1.261E44	6h
cce@8.5.5	High	2.272E46	1.341E44	5h



**TEN YEARS REPRODUCIBILITY CHALLENGE**  
RESCIENCE SPECIAL ISSUE  
FREE TO READ - FREE TO PUBLISH

Would you dare to run the code from your past self?  
(the one that does not answer mail)

SUBMISSION DEADLINE 01/04/2020  
<http://rescience.github.io/ten-years>  
In association with Inria, CNRS, Software Heritage, REScience, Comité pour la Science Ouverte,  
URFCI Bordeaux à l'occasion de la journée et du numérique pour l'enseignement supérieur.

<http://rescience.github.io/ten-years/>

```
import matplotlib
print(matplotlib.__version__)
```

3.1.2

```
import matplotlib
print(matplotlib.__version__)
```

## 3.1.2

```
apt show python3-matplotlib
```

Package: python3-matplotlib

Version: 3.1.2-2

Priority: optional

Section: python

Source: matplotlib

Maintainer: Sandro Tosi <morph@debian.org>

Installed-Size: 15.3 MB

Depends: python3-dateutil, python-matplotlib-data (>= 3.1.2-2), python3-pyparsing (>= 1.4), libjs-jquery, libjs-jquery-ui, python3-numpy (>= 1:1.16.0~rc1), python3-numpy-abi9, python3 (<< 3.9), python3 (>= 3.7~), python3-cycler (>= 0.10.0), python3-kiwisolver, python3:any, libc6 (>= 2.29), libfreetype6 (>= 2.2.1), libgcc-s1 (>= 3.0), libpng16-16 (>= 1.6.2-1), libstdc++6 (>= 5.2)

Recommends: python3-pil, python3-tk

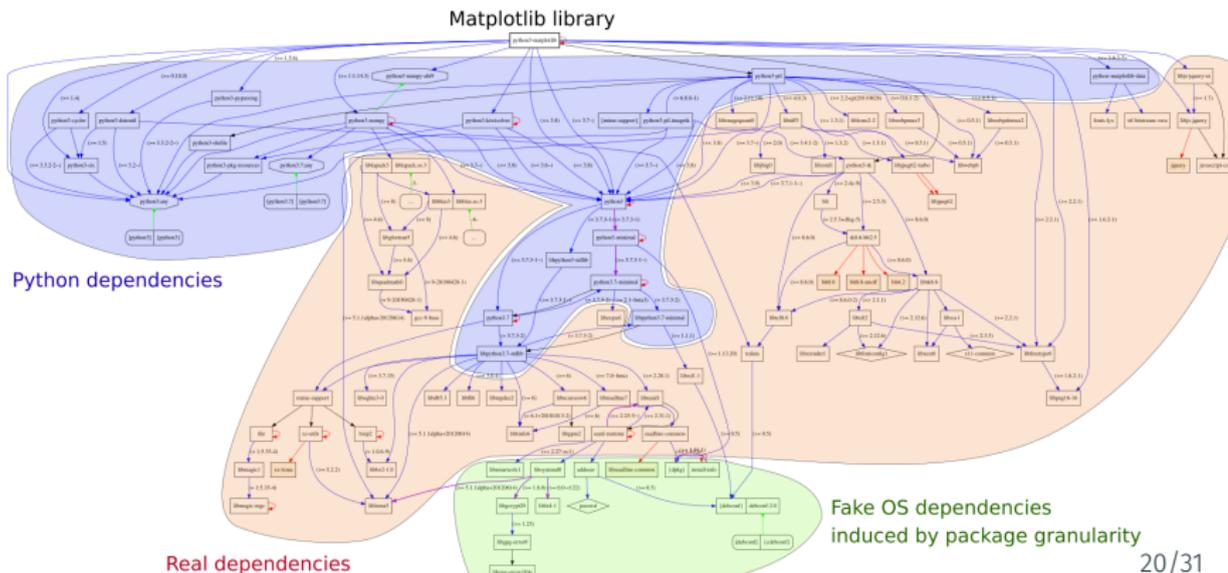
Suggests: dvipng, ffmpeg, gir1.2-gtk-3.0, ghostscript, inkscape, ipython3, librsvg2-common, python-matplotlib-doc, python3-cairocffi, python3-gi, python3-gi-cairo, python3-gobject, python3-nose, python3-pyqt5, python3-scipy, python3-sip, python3-tornado, python3-tornadoc, texlive-extra-utils, texlive-latex-extra, ttf-staypuft

# COMPLEX ECOSYSTEMS

```
import matplotlib  
print(matplotlib.__version__)
```

## 3.1.2

```
apt show python3-matplotlib
```



# NON STANDARD ECOSYSTEMS

## No standard

- Linux (`apt`, `rpm`, `yum`), MacOS X (`brew`, `MacPorts`, `Fink`), Windows (?)
- Neither for installation nor for retrieving the information... 😞

```
import sys
print(sys.version)
import matplotlib
print(matplotlib.__version__)
import pandas as pd
print(pd.__version__)
```

```
3.7.6 (default, Jan 19 2020, 22:34:52)
[GCC 9.2.1 20200117]
3.1.2
0.25.3
```

```
library(ggplot2)
sessionInfo()
```

```
R version 3.6.3 RC (2020-02-21 r77847)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Debian GNU/Linux bullseye/sid

Matrix products: default
BLAS: /usr/lib/x86_64-linux-gnu/atlas/libblas.so.3.10.3
LAPACK: /usr/lib/x86_64-linux-gnu/atlas/liblapack.so.3.10.3

locale:
 [1] C

attached base packages:
 [1] stats      graphics  grDevices  utils      datasets  method

other attached packages:
 [1] ggplot2_3.2.1

loaded via a namespace (and not attached):
 [1] Rcpp_1.0.3      withr_2.1.2     crayon_1.3.4    dplyr
 [5] assertthat_0.2.1 grid_3.6.3      R6_2.4.1        life
 [9] gtable_0.3.0   magrittr_1.5    scales_1.1.0    pill
[13] rlang_0.4.4    lazyeval_0.2.2 glue_1.3.1      purr
[17] munsell_0.5.0  compiler_3.6.3 pkgconfig_2.0.3 tibble
[21] tidyselect_1.0.0 tibble_2.1.3
```

# ARGH... DAMNED COMPUTERS

- Whenever I upgrade my computer, things break so I try to stay away from this 😞
- Whenever trying the code of my colleague, I had to install Foo but I broke everything and now neither his code nor mine works! 😞
- But hey! Here is my code, feel free to play with it! I'm doing open science 😊

Are you really aware of your dependencies ?

- No one will ever run/use your code if it isn't easy to install
- No one will ever manage to run your code if you don't document how to run it
- Others (even you) are unlikely to get the same results unless you automate the execution

## TOOL 2: CONTAINERS AND PACKAGE MANAGERS

The good



Automatic tracking

The bad



The ugly



## TOOL 2: CONTAINERS AND PACKAGE MANAGERS



Automatic tracking

Containers

- **Pros:** Lightweight, Good isolation, Easy to use
  - Running as easy as `docker run <img> <cmd>`
  - Building images: `docker build -f <Dockerfile>`
  - Sharing through the **Docker Hub**: `docker pull/push <img>`

## TOOL 2: CONTAINERS AND PACKAGE MANAGERS



Automatic tracking

Containers

- **Pros:** Lightweight, Good isolation, Easy to use
- **Cons:** Opaque, Container build is generally not reproducible
  - Recipes rarely follow *reproducible good practices*

```
FROM ubuntu:20.04
RUN apt-get update
    && apt-get upgrade -y
    && apt-get install -y ...
```

- Choose a stable image (and the smallest possible)
- Include only the necessary libraries (e.g. no graphics libs)
- Avoid system updates (instead freeze sources)

## TOOL 2: CONTAINERS AND PACKAGE MANAGERS



Automatic tracking

Containers

- **Pros:** Lightweight, Good isolation, Easy to use
- **Cons:** Opaque, Container build is generally not reproducible

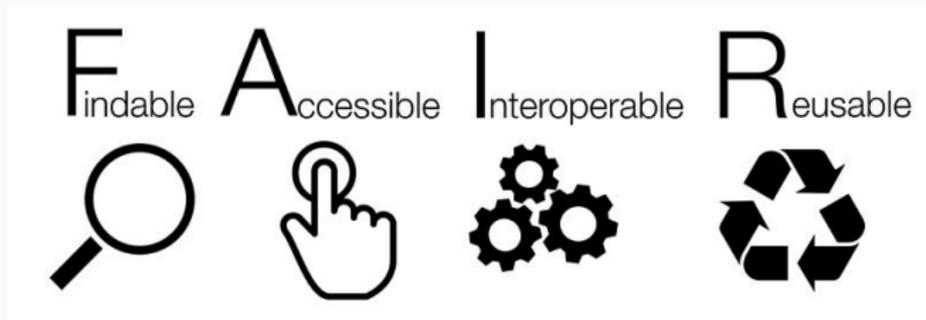
Package managers

- Language specific: **pip/pipenv/virtualenv, conda, CRAN/Bioconductor**
  - **Limits:** version management, durability, permeable, language centric
- **GUIX/NiX** = Full-fledged functional package manager
  - Native support for environment (*à la git*)
  - Isolation through **--pure**
  - Recompile from source (cache recommended)

GOOD PRACTICE #3

VERSION CONTROL AND ARCHIVING

---



<https://www.go-fair.org/fair-principles/>

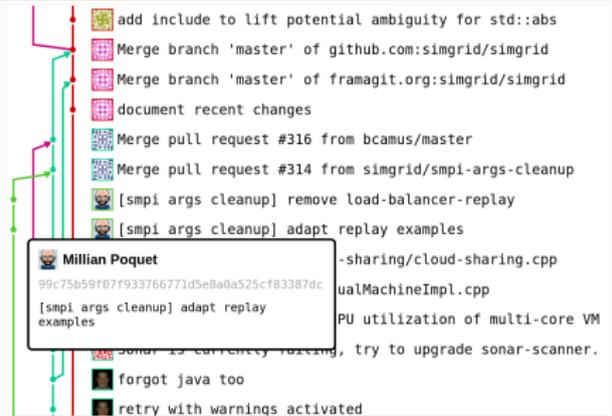
- *"Open as much as possible and close as much as necessary"*
- Management, publication, annotation (metadata), archiving
- Source code = specific data with specific consideration

Let's go beyond general principles!

# TOOL 3: VERSION CONTROL AND FORGE

## Git = version control

- Developed in 2005 by Linus Torvalds for the kernel development
- Local and efficient rollbacks
- Distributed: everyone has a full copy of the history



## GitHub, GitLab, and Co

- Free hosting of public projects, social network
- Web interfaces (browsing, preview, online editing)
- User management (read/write, public/private)
- Issues, Continuous Integration, ...



## TOOL 3BIS: FIGHTING INFORMATION LOSS WITH ARCHIVES



or



= awesome collaborations ( $\neq$  archive)

- D. Spinellis. *The Decay and Failures of URL References*. CACM, 46(1), 2003  
*The half-life of a referenced URL is approximately 4 years from its publication date.*
- P. Habibzadeh. *Decay of References to Web sites in Articles Published in General Medical Journals: Mainstream vs Small Journals*. Applied Clinical Informatics. 4 (4), 2013  
*half life ranged from 2.2 years in EMHJ to 5.3 years in BMJ*
- Discontinued forges: Code Space, Gitorious, Google code, Inria Gforge

# TOOL 3BIS: FIGHTING INFORMATION LOSS WITH ARCHIVES



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



Data archives



Software Archive



Software Heritage

Collect/Preserve/Share



WHAT WILL IT TAKE ?

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## 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



**Learn and Teach** using online resources like

- **Software Carpentry**, **The Turing Way**, ...

## 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...

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

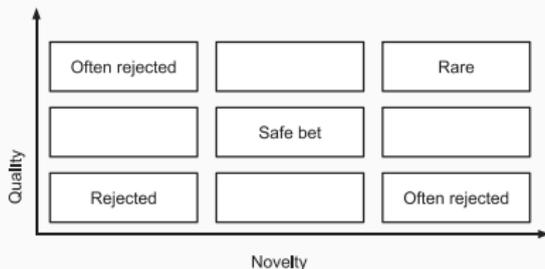
# CHANGING ACADEMIC PRACTICES (PUBLISH OR PERISH)

- **Goodhart's Law: Are Academic Metrics Being Gamed?**, M. Fire 2019
  - AI: over 1,000 ranked journals ( $\times 10$  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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- **The Truth, The Whole Truth, and Nothing But the Truth: A Pragmatic, Guide to Assessing Empirical Evaluations**, *TOPLAS* 2016



- **Impact factor abandoned by Dutch university in hiring and promotion, decisions.** *Nature*, June 2021. *Faculty and staff members at Utrecht University will be evaluated by their commitment to open science*

# WHAT ABOUT OPEN SCIENCE ?

## Plan National pour la Science Ouverte (BSN $\rightsquigarrow$ 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 (avoid **collusion**)
6. Open educational resources





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

- Loïc Desquilbet, Sabrina Granger, Boris Hejblum, Pascal Pernot, Nicolas Rougier

# RESOURCES AND ACKNOWLEDGMENTS



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

- Loïc Desquilbet, Sabrina Granger, Boris Hejblum, Pascal Pernot, Nicolas Rougier

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

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

