

# REPRODUCIBILITY CRISIS, OPEN SCIENCE,... AND COMPUTER SCIENCE

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Arnaud Legrand



LISTIC, Annecy  
February 2023



# WHAT IS SCIENCE?

Question 1: In less than 5 lines give a definition of "Science"

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## Dictionary of science and technology

1. the study of the physical and natural world and phenomena, especially by using systematic observation and experiment
2. a particular area of study or knowledge of the physical world
3. a systematically organized body of knowledge about a particular subject

**New Oxford Dictionary** the intellectual and practical activity encompassing the systematic study of the structure and behavior of the physical and natural world through observation and experiment : the world of science and technology.

1. a particular area of this : veterinary science | the agricultural sciences.
2. a systematically organized body of knowledge on a particular subject : the science of criminology.
3. archaic knowledge of any kind.

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1. a particular area of this : veterinary science | the agricultural sciences.
2. a systematically organized body of knowledge on a particular subject : the science of criminology.
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**Building Reliable Knowledge**

# 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

Los Angeles Times | BUSINESS

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.

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More > Science Magazine > 22 MARCH 2012 > MONDAY, 24 (160) : 229  
Article Views Science 17 January 2014;  
Summary Vol. 343 no. 6168 p. 229  
DOI: 10.1126/science.1250475  
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24 April 2013



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Must try harder  
Nature 483, 509 (29 March 2012) doi:10.1038/483509a  
Published online: 28 March 2012  
PDF Cite This Email Reprints Rights & permissions Article metrics  
Too many sloppy mistakes are creeping into scientific papers. Lab heads must look more rigorously at the data — and at themselves.

TheScientist EXPLORING LIFE. INSPIRING INNOVATION

NIH Tackles Irreproducibility

The federal agency speaks out about how to improve the quality of scientific research.

By Jef Akst | 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
- 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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**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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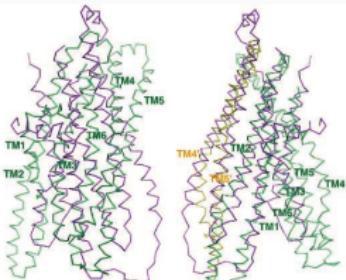
## Bad science is deleterious

- 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!*

# How COMPUTERS BROKE SCIENCE



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

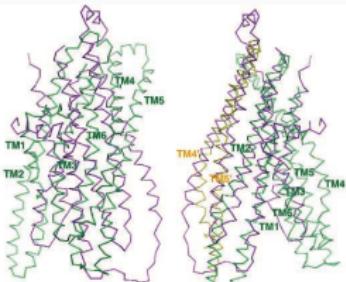
He specialized in structures of **multidrug resistant transporter proteins in bacteria**: MsbA de Escherichia Choli (Science, 2001), Vibrio cholera (Mol. Biology, 2003), Salmonella typhimurium (Science, 2005)

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 retractions** that motivate **improved software engineering practices** in comp. biology

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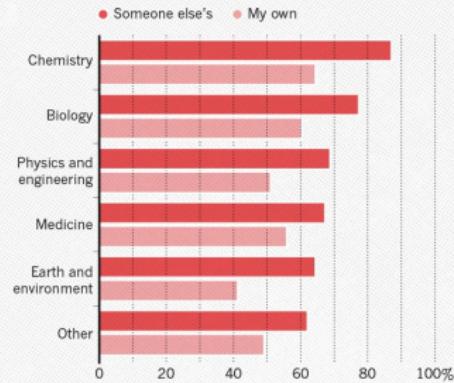
There is **worse!**

- 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

# A REPRODUCIBILITY CRISIS?

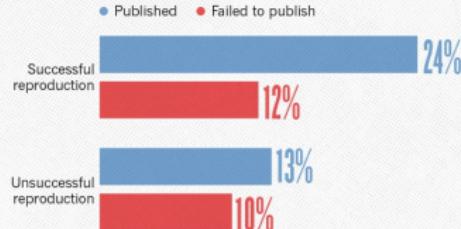
## HAVE YOU FAILED TO REPRODUCE AN EXPERIMENT?

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.



1,500 scientists lift the lid on reproducibility,

Nature, May 2016

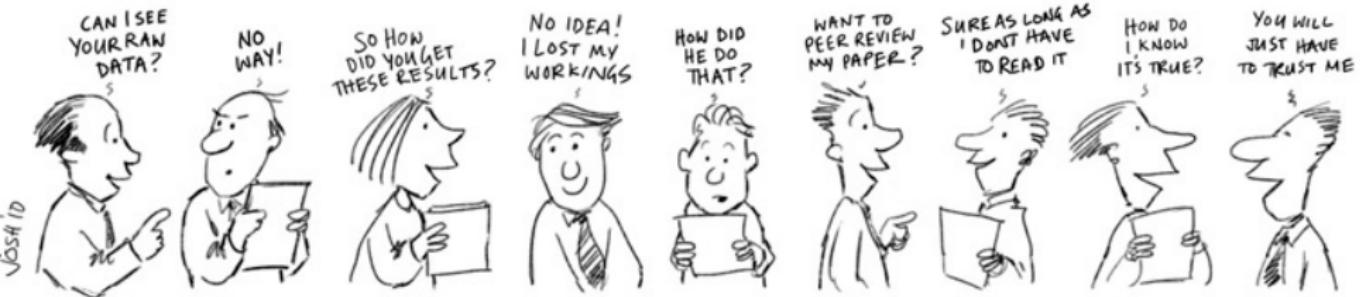
## Social causes

- 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

# NO TRANSPARENCY NO CONSENSUS



# DIFFERENT REPRODUCIBILITY CONCERN IN MODERN SCIENCE

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

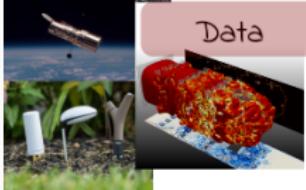
**Genomics** software engineering, computational reproducibility, provenance

**Computational fluid dynamics** numerical issues

**Artificial Intelligence** most of the above

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

## Authors



Data

# DIFFERENT REPRODUCIBILITY CONCERN IN MODERN SCIENCE

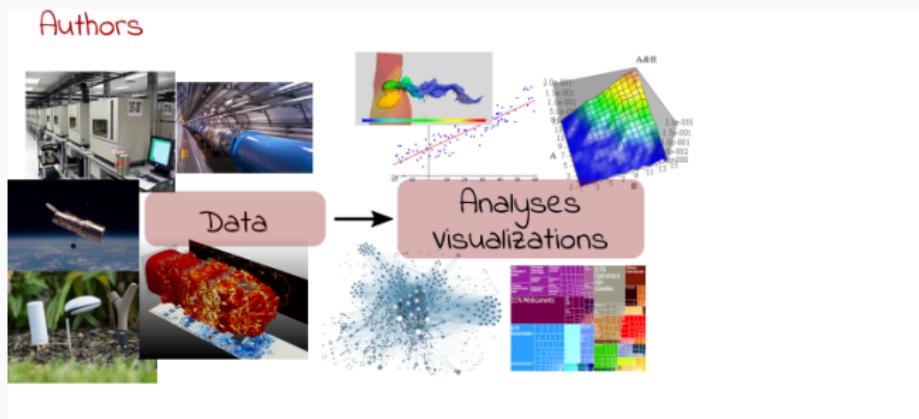
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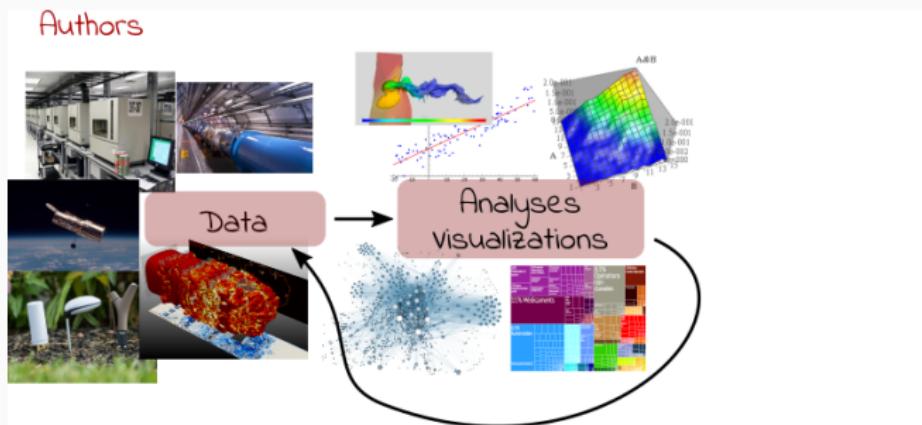
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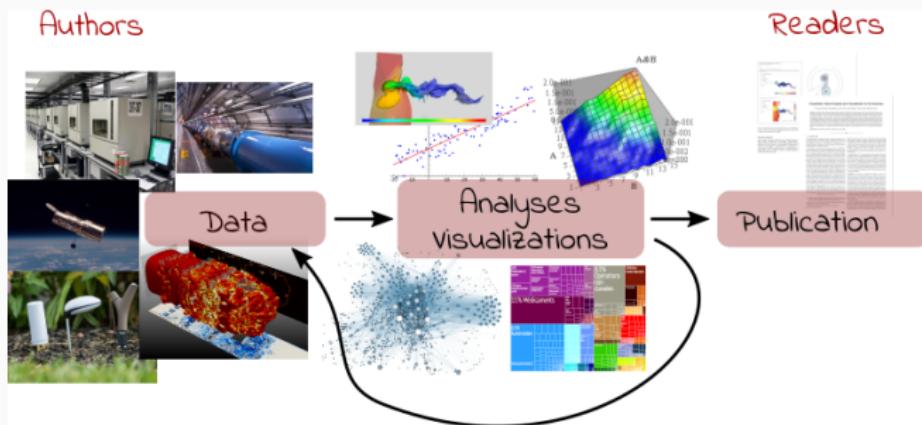
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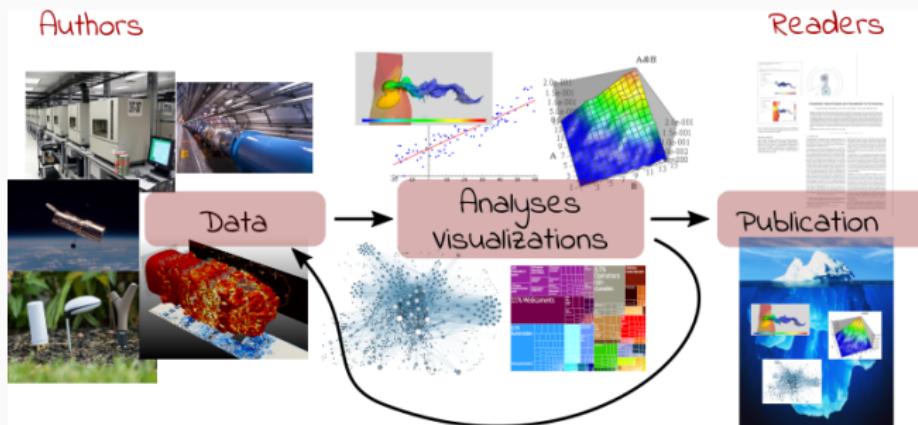
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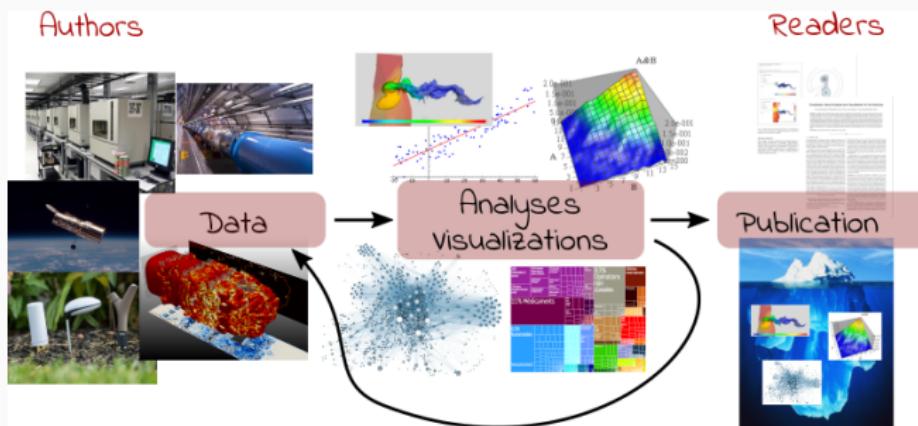
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Reproducible Research = Bridging the Gap by working Transparently 8/100

# REPRODUCIBLE RESEARCH PRACTICES

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# 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. Durrif, 2021

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

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

<sup>3</sup>Bitwise

# "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 documents.

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).

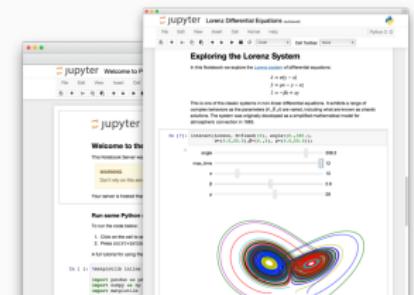
- make incremental improvements in electronic-document software
- seek partners for broadening standards (and making incremental improvements).

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.

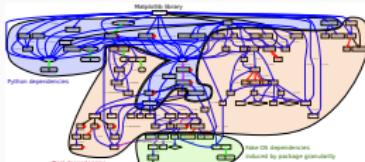
Now that we have begun using CD-ROM publication, we can go much further. Every figure caption contains a pushbutton that jumps to the appropriate science directory (folder) and initiates a figure rebuild command and then displays the figure, possibly as a movie or interactive program. We normally display 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 L<sup>A</sup>T<sub>E</sub>X word processing systems. Naturally some software includes licensed software, but with the exception

# EXISTING TOOLS, EMERGING STANDARDS

## Notebooks and workflows



## Software environments



## Sharing platforms



## GOOD PRACTICE #1

### TAKING NOTES AND DOCUMENTING

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## 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

# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Un document computationnel

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

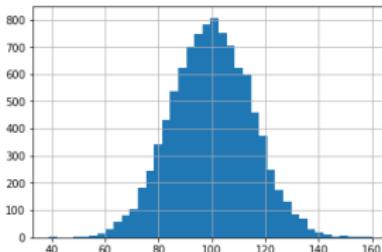
3.141592653589793

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 details:

- Title:** # Un document computationnel
- In [1]:** A code cell containing:

```
from math import *
print(pi)
3.141592653589793
```
- Out [1]:** The output 3.141592653589793, followed by a note: "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 obtientrait comme approximation :".
- In [2]:** A code cell containing:

```
import numpy as np
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theta = np.random.uniform(size=N, low=0, high=np.pi/2)
2/(sum((x+np.sin(theta))>1))/N
```
- Out [2]:** The output 3.14371986944998765, followed by a note: "On peut inclure des formules mathématiques comme  $\sqrt{2/\pi} \exp(-x^2/2)$  et des dessins qui n'ont rien à voir avec  $\pi$  (si ce n'est une constante de normalisation...)."
- In [3]:** A code cell containing:

```
%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()
```
- Out [3]:** A histogram showing a bell-shaped distribution centered around 100.

Document final

## Un document computationnel

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

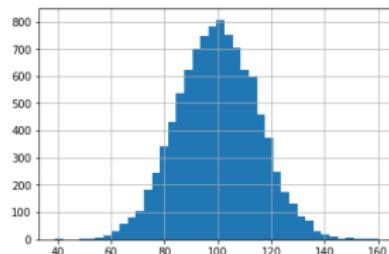
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Document initial dans son environnement

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

In [1]: from math import * print(pi)
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Mais calculé avec la méthode des aiguilles de Buffon (https://fr.wikipedia.org/wiki/Aiguille\_de\_Buffon), on obtient aussi comme approximation : 3.141592653589793

In [2]: N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=np.pi/2)
2*(sum((x+np.sin(theta))>1))/N
Out[2]: 3.14371986944998765

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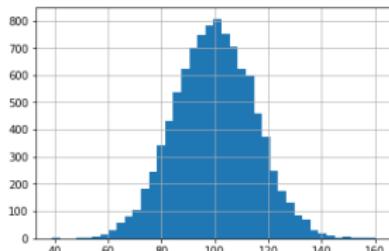
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Mais calculé avec la [méthode des aiguilles de Buffon](#), on obtient comme approximation :

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# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

Document initial dans son environnement

A screenshot of a Jupyter Notebook interface. The top bar shows 'jupyter example\_pi' and 'Python 3'. The notebook contains three code cells:

- In [1]:** Prints the value of pi calculated using the formula  $\frac{2 \times \text{count}}{\text{N}}$ . It also links to a Wikipedia page on the method.
- In [2]:** Calculates the same value using a different approach involving sine and uniform distribution.
- In [3]:** Plots a histogram of 100,000 random numbers between 0 and 160, showing a bell-shaped distribution centered around 100.

Red arrows point from the text 'Code' and 'Un document computationnel' to the code cells in the Jupyter interface.

Document final

## Un document computationnel

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

3.141592653589793

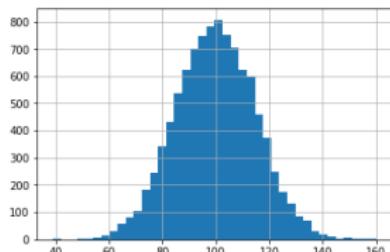
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```
import numpy as np
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2 * (sum((x+np.sin(theta))>1))/N
```

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... ☺).



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3,141592653589793
```

Mais calculé avec la `_methode_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  
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  
Out[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  
import matplotlib.pyplot as plt  
  
mu, sigma = 100, 15  
x = mu + sigma*np.random.randn(10000)  
  
plt.hist(x, 99)  
plt.grid(True)  
plt.show()
```

Document final

## Un document computationnel

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

3.141592653589793

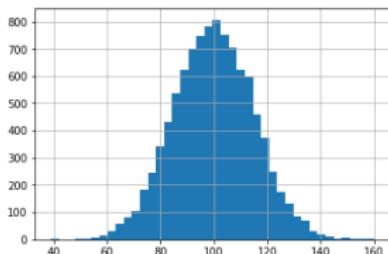
Mais calculé avec la méthode des aiguilles de Buffon, on obtiendrait comme approximation :

```
import numpy as np  
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 three code cells:

- In [1]:** Prints the value of pi (3.141592653589793) and includes a note about calculating pi using Buffon's needle method.
- In [2]:** Generates a uniform distribution of points (x, theta) and calculates an approximation of pi based on the ratio of points falling within a quarter circle.
- In [3]:** Plots a histogram of x values, showing a normal distribution centered around 100.

Document final

## Un document computationnel

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

3.141592653589793

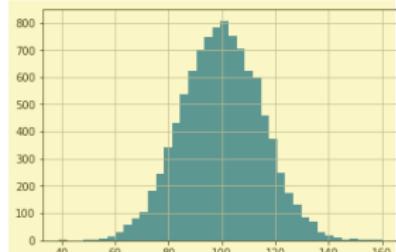
Mais calculé avec la méthode des [aiguilles de Buffon](#), on obtiendrait comme approximation :

```
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

Export

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 several code cells:

- In [1]:** `# Un document computationnel`  
Output: `Mon ordinateur m'indique que $\pi$ vaut "approximativement"`  
Code:

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

Output: `3.141592653589793`
- In [2]:** `Mais calculé avec la __method__ des "épaulette de Buffon"`  
[https://fr.wikipedia.org/wiki/Alg\u00fclie\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Alg\u00fclie_de_Buffon), on obtiendrait comme approximation :  
Code:

```
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)
```

Output: `3.1437198694098765`
- In [3]:** `On peut inclure des formules math\u00e9matiques comme $\\frac{1}{\\sigma\\sqrt{2\\pi}} \\exp\\left(-\\frac{(x-\\mu)^2}{2\\sigma^2}\\right)$ et des dessins qui n'ont rien \u00e0 voir avec $\\pi$ (si ce n'est une constante de normalisation...).`  
Code:

```
%matplotlib inline
import matplotlib.pyplot as plt
mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)
plt.hist(x,99)
plt.grid(True)
plt.show()
```



Document final

## Un document computationnel

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

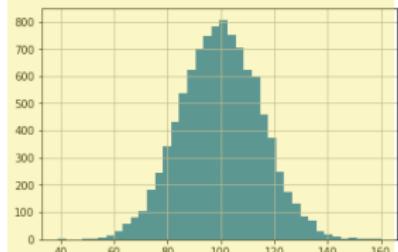
3.141592653589793

Mais calcul\u00e9 avec la **m\u00e9thode des aiguilles de Buffon**, on obtiendrait comme approximation :

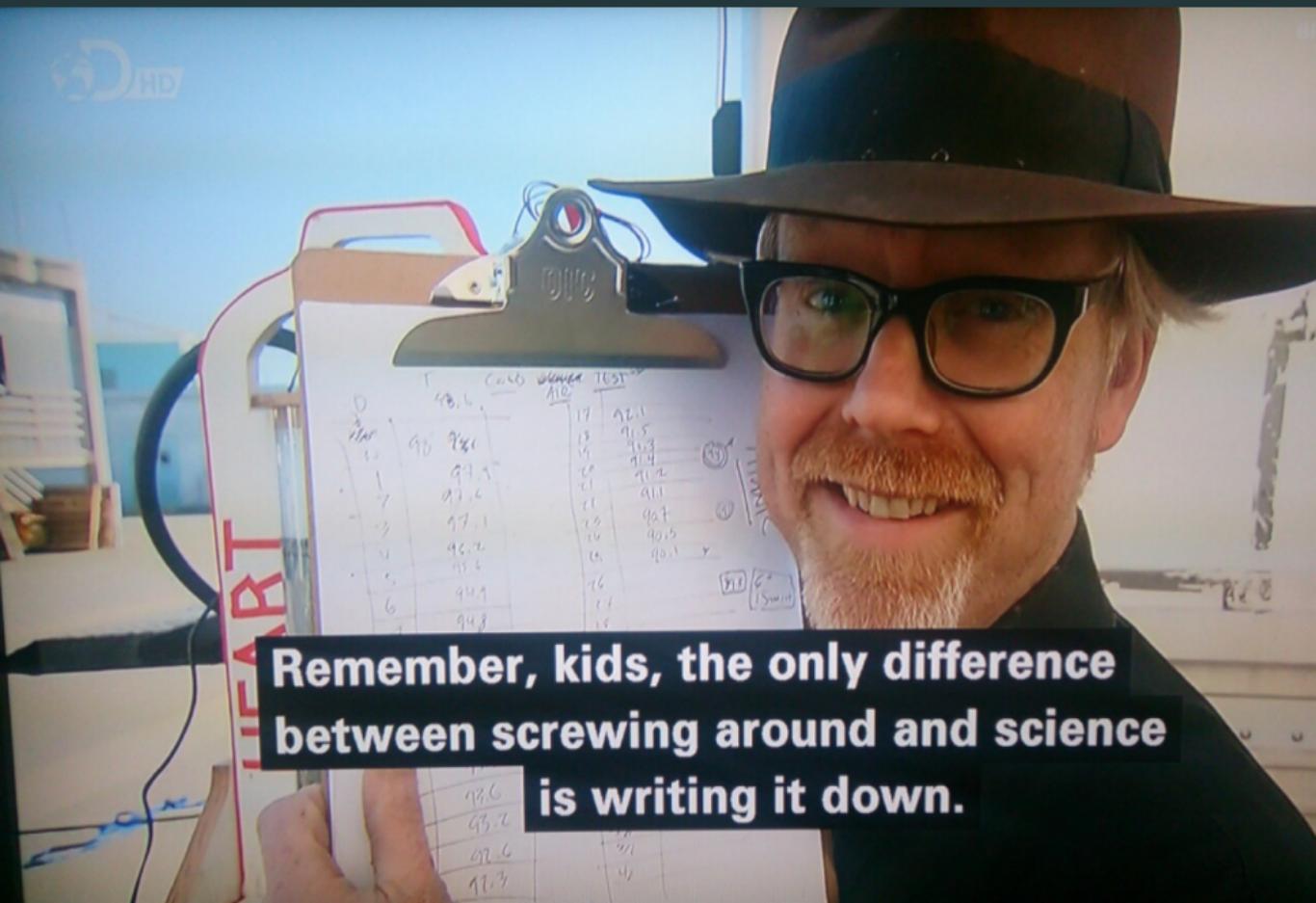
```
import numpy as np
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1)/N)
```

3.1437198694098765

On peut inclure des formules math\u00e9matiques comme  $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$  et des dessins qui n'ont rien \u00e0 voir avec  $\pi$  (si ce n'est une constante de normalisation...).



## TOOL 1 BIS: LABORATORY NOTEBOOKS, COMPUTATIONAL DOCUMENTS



**Remember, kids, the only difference  
between screwing around and science  
is writing it down.**

# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

jupyter example\_pi [recent]

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

# Un document computationnel

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

In [1]:

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

Mais calculé avec la `__method__` des (ajoutées de Buffet) `__approximation__`, on obtiendrait comme

In [2]:

```
import numpy as np  
n = 1000000  
x = np.random.uniform(0, low=0, high=1)  
theta = np.random.uniform(0, low=0, high=np.pi/2)  
if (x**2 + np.sin(theta)**2) < 1/n
```

Out[2]: 3.1437198684950785

On peut inclure des formules mathématiques comme  $\frac{1}{\sqrt{\pi}}$  via `mathop` ou `math`. Cela nous permet de dessiner ce qu'il est rien à voir avec `math` (si ce n'est une constante de normalisation...).

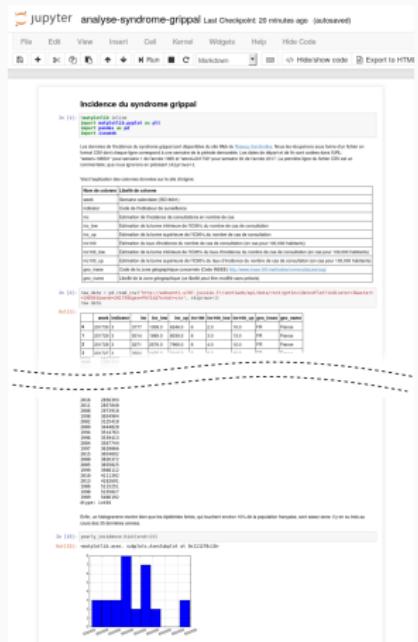
In [3]:

```
%matplotlib inline  
import matplotlib.pyplot as plt  
  
N = sigma = 100, 33  
x = mu = np.linspace(-random.randrange(10000),  
plt.hist(x, 40)  
plt.title("sigma = %d" % sigma)  
plt.show()
```



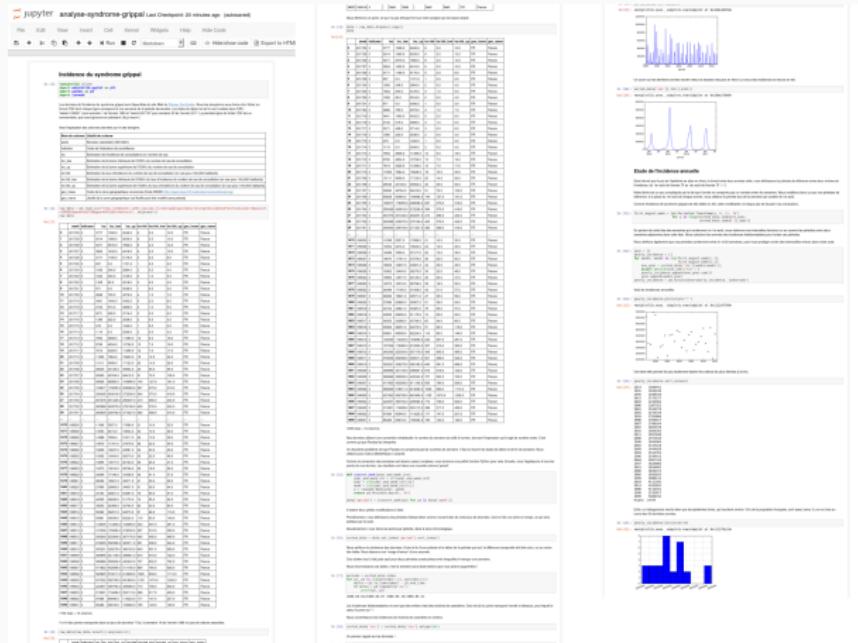
## TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code



# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code



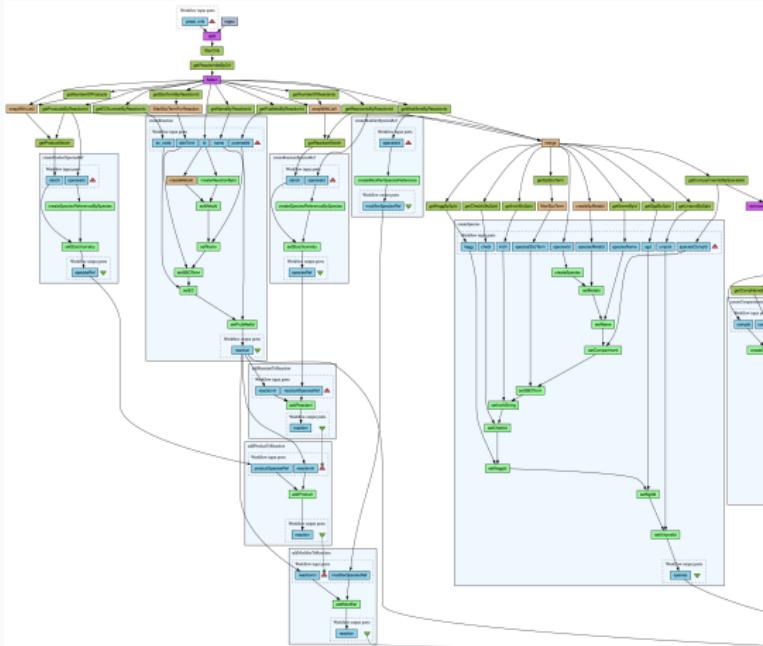
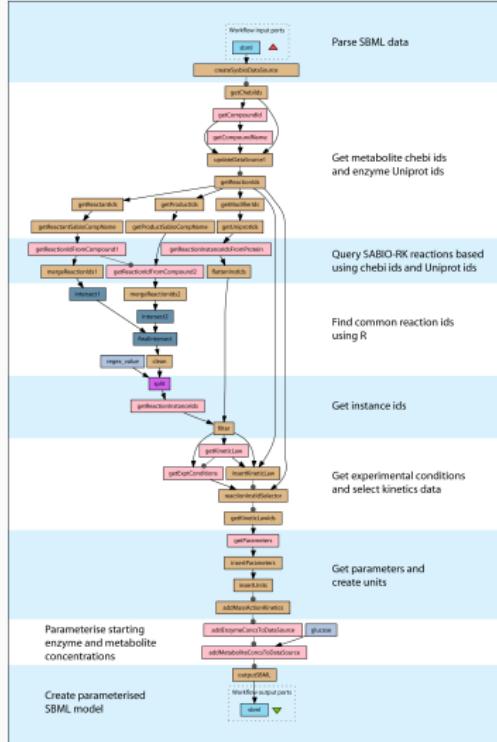
# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

The image displays a 4x3 grid of Jupyter Notebook screenshots, each illustrating a different step or aspect of a workflow. The notebooks cover topics such as estimating color names from web images, performing k-means clustering, visualizing color distributions, and analyzing machine learning model results.

- Row 1:**
  - Estimating Color Names by Web Image**: A notebook cell with code and a warning about the complexity of the task.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of k-means clustering on a dataset of 1000 images.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 2:**
  - Dimensionality reduction**: A notebook cell with code and a note about the curse of dimensionality.
  - Dimensionality reduction**: A notebook cell showing the implementation of PCA.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
- Row 3:**
  - PCA**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - PCA**: A notebook cell with code and a note about PCA being orthogonal.
- Row 4:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Prediction**: A notebook cell with code and a note about PCA being orthogonal.
- Row 5:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a scatter plot titled "Chromaticity distribution of training data" with axes "L\* value" and "a\* value".
- Row 6:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 7:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 8:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 9:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 10:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 11:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.
- Row 12:**
  - Dimensionality reduction**: A notebook cell with code and a note about PCA being orthogonal.
  - Dimensionality reduction and k-means**: A notebook cell showing the implementation of PCA followed by k-means clustering.
  - Dimensionality reduction and k-means results**: A notebook cell displaying a heatmap titled "Color space" with a color bar and numerical values.

# TOOL 1 TER: WORKFLOWS



## TOOL 1 TER: WORKFLOWS

### Workflows:

- Clearer high-level view
- **Explicit** composition of codes and data movement
- 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: `make`, dask, drake, swift, `snakemake`, ...
- Hybrids: SOS-notebook, ...

## GOOD PRACTICE #2

### CONTROLLING SOFTWARE ENVIRONMENT

---

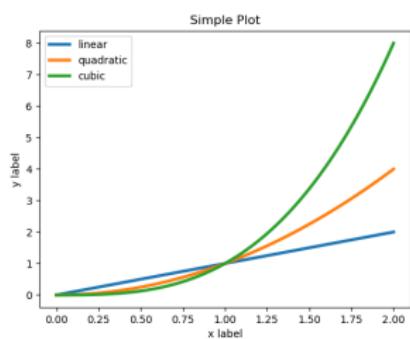
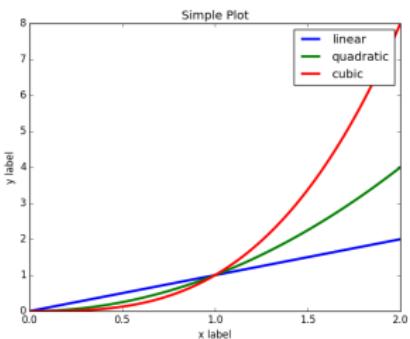
## ARGH... DAMNED COMPUTERS

- 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 😞
  - Whenever trying the code of my colleague, I had to install **libFoo-1.5c** but I broke everything and now neither his code nor mine works! 😞
  - But hey! Here is my code. It's on GitHub so feel free to play with it! I'm doing open science 😊
    1. No one will ever run/use your code if it isn't easy to install
    2. No one will ever manage to run your code if you don't document how to run it
    3. Others (even you) are unlikely to get the same results unless you control and share your software environment

## SOFTWARE DEPENDENCIES: HORROR STORIES

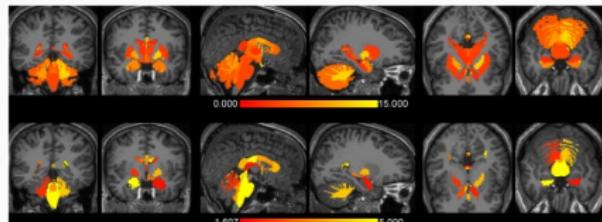
# SOFTWARE DEPENDENCIES: HORROR STORIES

- Software environment evolution



# SOFTWARE DEPENDENCIES: HORROR STORIES

- Software environment evolution
- 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:*

- volume:  $8.8 \pm 6.6\%$  (range 1.3-**64.0%**)
- cortical thickness:  $2.8 \pm 1.3\%$  (range 1.1-7.7%)

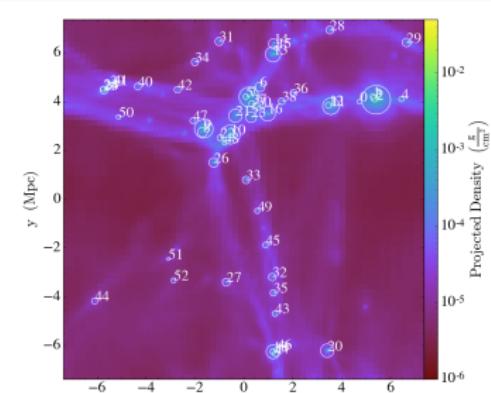
*About a factor two smaller differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

*In the context of an ongoing study, users are discouraged to update to a new major release of either FreeSurfer or operating system.*

*Formal assessment of the accuracy of FreeSurfer is desirable.*

# SOFTWARE DEPENDENCIES: HORROR STORIES

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

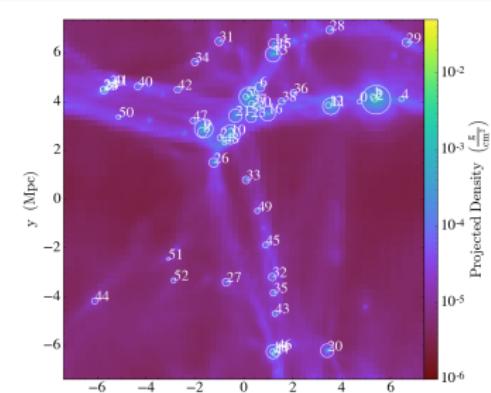


Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

Compiler	Optim.	Largest Halo Avg Mass.	Std. Err	Walltime
gcc@6.2.0	None	2.273E 46	1.069E 44	22h

# SOFTWARE DEPENDENCIES: HORROR STORIES

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

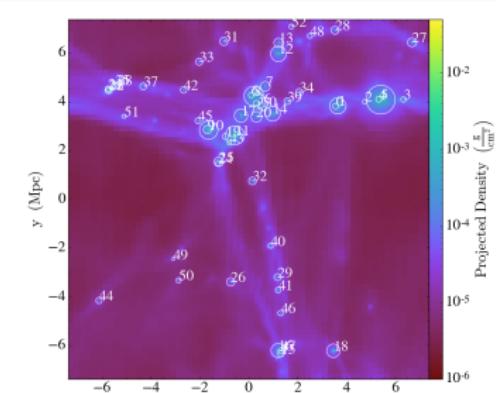


Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

Compiler	Optim.	Largest Halo Avg Mass.	Std. Err	Walltime
gcc@6.2.0	None	2.273E 46	1.069E 44	22h

# SOFTWARE DEPENDENCIES: HORROR STORIES

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

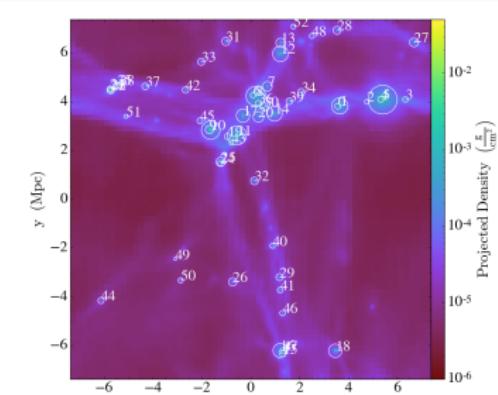


Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

Compiler	Optim.	Largest Halo		Walltime
		Avg Mass.	Std. Err	
gcc@6.2.0	None	2.273E 46	1.069E 44	22h
gcc@6.2.0	Normal	2.266E 46	1.218E 44	10h
gcc@6.2.0	High	2.275E 46	1.199E 44	9h

# SOFTWARE DEPENDENCIES: HORROR STORIES

- Software environment evolution
  - 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	2.273E 46	1.069E 44	22h
gcc@6.2.0	Normal	2.266E 46	1.218E 44	10h
gcc@6.2.0	High	2.275E 46	1.199E 44	9h
intel@16.0.3	None	<b>22.71</b> E 46	1.587E 44	39h
intel@16.0.3	Normal	<b>43.30</b> E 46	1.248E 44	7h
intel@16.0.3	High	2.268E 46	1.414E 44	6h
cce@8.5.5	Low	<b>43.11</b> E 46	1.353E 44	16h
cce@8.5.5	Normal	2.271E 46	1.261E 44	6h
cce@8.5.5	High	2.272E 46	1.341E 44	5h

# COMPLEX ECOSYSTEMS

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

3.5.1

# COMPLEX ECOSYSTEMS

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

## 3.5.1

```
1 apt show python3-matplotlib
```

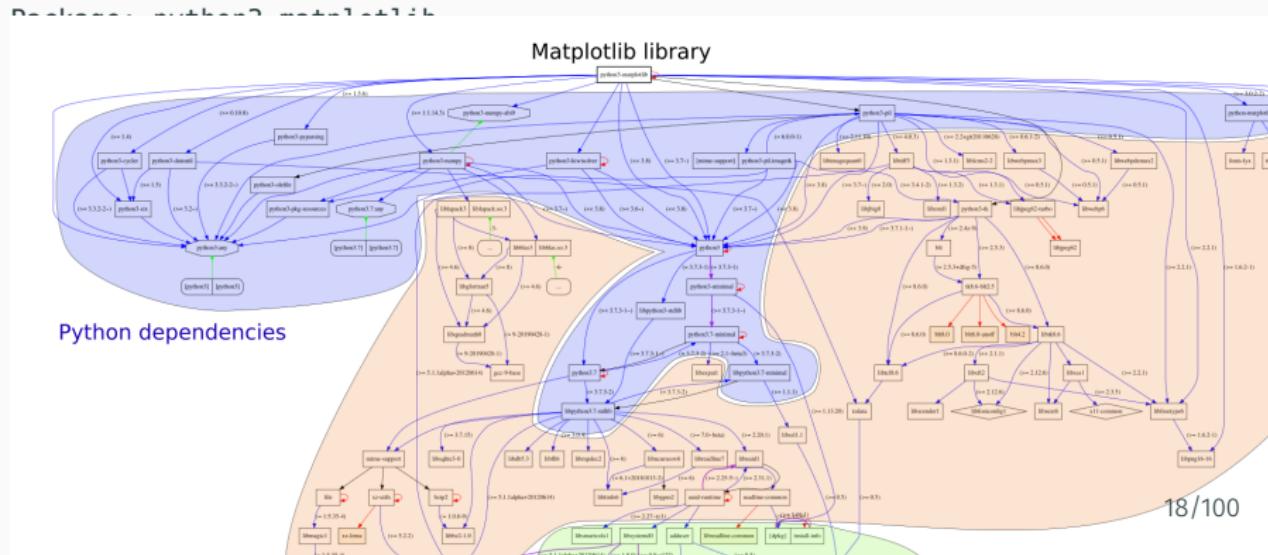
Package: python3-matplotlib  
Version: 3.5.1-2+b1  
Source: matplotlib (3.5.1-2)  
Maintainer: Sandro Tosi <morph@debian.org>  
Installed-Size: 27.6 MB  
Depends: libjs-jquery, libjs-jquery-ui, python-matplotlib-data (>= 3.5.1),  
 python3-dateutil, python3-pil.imagetk, python3-pyparsing (>= 1.5.6),  
 python3-six (>= 1.4), python3-numpy (>= 1:1.20.0), python3-numpy-  
 abi9,  
 python3 (<< 3.11), python3 (>= 3.9~), python3-cycler (>= 0.10.0),  
 python3-fonttools, python3-kiwisolver, python3-packaging, python3-  
 pil,  
 python3:any, libc6 (>= 2.29), libfreetype6 (>= 2.2.1),  
 libgcc-s1 (>= 3.3.1), libqhull-r8.0 (>= 2020.1), libstdc++6 (>= 11)  
Recommends: python3-tk  
Suggests: dvipng, ffmpeg, fonts-staypuft, ghostscript, gir1.2-gtk-3.0, inkscape,

## COMPLEX ECOSYSTEMS

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

### 3.5.1

```
1 apt show python3-matplotlib
```



## TOOL 2: CONTAINERS AND PACKAGE MANAGERS

The good



The bad



The ugly



Automatic tracking

## TOOL 2: CONTAINERS AND PACKAGE MANAGERS

The good



The bad



The ugly



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

The good



The bad



The ugly



Automatic tracking

### Containers

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

```
1   FROM ubuntu:20.04
2   RUN apt-get update
3       && apt-get upgrade -y
4       && 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

The good



The bad



The ugly



Automatic tracking

Containers

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

Package managers (the ugly and the good)

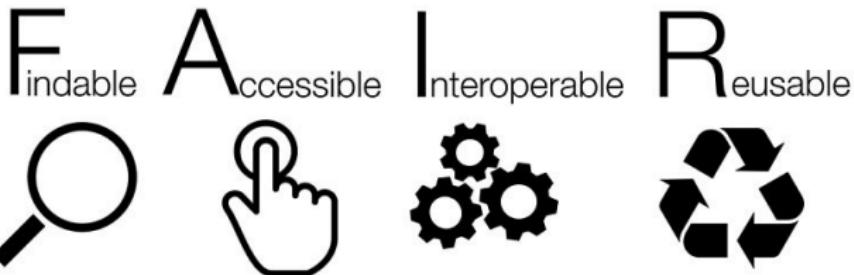
- Language specific: `pip/pipenv/virtualenv`, `conda`, `CRAN/Bioconductor`
  - Limits: version management, durability, permeable, language centric
- **GUIX/NiX** = Full-fledged functional package manager
  - Native support for environment (*à la git*)
  - Isolation through `--pure`
  - Recompile from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

## GOOD PRACTICE #3

### VERSION CONTROL AND ARCHIVING

---

# FAIR PRINCIPLES



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

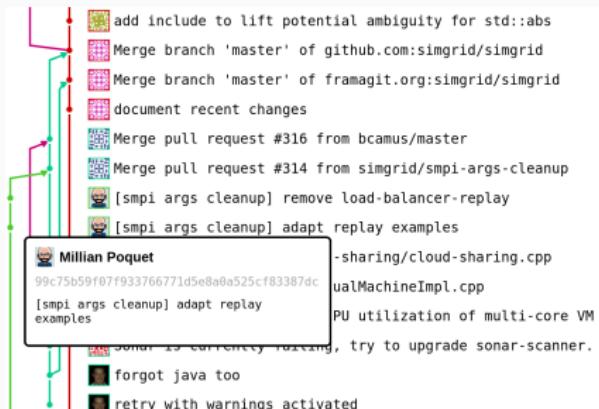
- "*Open as much as possible and close as much as necessary*"
- Management, publication, annotation (metadata), archiving
- Source code = specific data with specific consideration

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



## Limitation

- Managing large data: **Git LFS**   **Git Annex** (or DataLad)

## 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



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- D. Spinellis. *The Decay and Failures of URL References*. CACM, 46(1), 2003  
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*half life ranged from 2.2 years in EMHJ to 5.3 years in BMJ*
- Discontinued forges: Code Space, Gitorious, Google code, Inria Gforge

Article archives



Data archives



figshare



Software Archive



Software Heritage

Collect/Preserve/Share

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



Learn and Teach using online resources like

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

# 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



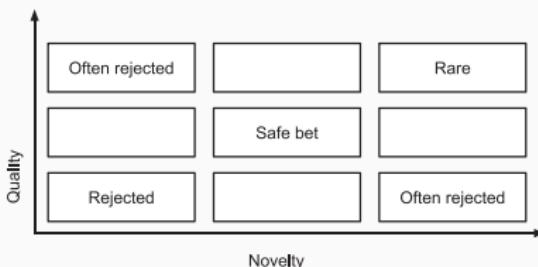
Joelle Pineau @ NeurIPS'18

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

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

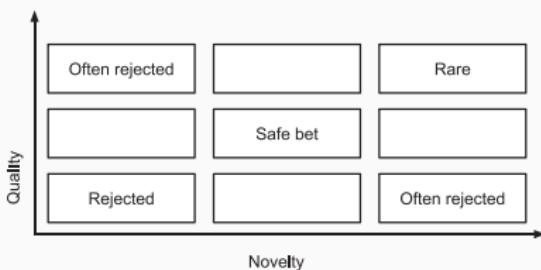
# CHANGING ACADEMIC PRACTICES (PUBLISH OR PERISH)

- 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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- 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 ~> 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



**NO TRANSPARENCY  
NO CONSENSUS**



THAT'S ALL FOLKS!

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# RESOURCES AND ACKNOWLEDGMENTS



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

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

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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 2023  
(15,000+)



Stay tuned for the MOOC "Advanced RR" planned for 2021 2022 2023

- Managing data (**FITS/HDF5, git annex**)
- Software environment control (**docker, singularity, guix**)
- Scientific workflow (**make, snakemake**)