

# REPRODUCIBILITY CRISIS AND OPEN SCIENCE

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Rencontres #FormIDEX, November 2019



# 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.

**Science** AAAS-ORG FEEDBACK HELP LIBRARAINS All Science Journals ▾ Search This Site

AAAS NEWS SCIENCE JOURNALS CAREERS MULTIMEDIA COLLECTIONS

Science The World's Leading Journal of Original Scientific Research, Global News, and Commentary.

Science Magazine > 22 JUNE 2013 > MONDAY, 24 JUNE (1660): 229

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### Editorial

#### Reproducibility

Marcia McNutt

► Marcia McNutt is editor-in-chief of *Science*.

Science advances on a foundation of trusted data. But a recent study found that the scientific community was shaken by reports that a troubling number of studies were irreproducible. For example, in one new meta-analysis, researchers found that only 11 percent of drug development studies fit one of the top recommendations of the U.S. National Institute of General Medical Sciences' "Guidelines for Increasing Transparency." Authors will indicate handling (such as how to deal with outliers), whether they used a sufficient signal-to-noise ratio, whether the experimenter was blind to the conduct of the experiments, and whether the results were statistically significant.

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

Announcement: Reducing our irreproducibility - Nature News & Comment

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nature International weekly journal of science

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Archive > Volume 490 > Issue 7446 > Editorial > Article

NATURE | EDITORIAL

### Announcement: Reducing our irreproducibility

24 April 2013

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Over the past year, *Nature* has published a string of articles that highlight the lack of reproducibility of published research (collected on

nature International weekly journal of science

Menu Advanced search Search

archive > volume 483 - issue 7591 - editorials - article

NATURE | EDITORIAL

### Must try harder

Nature 483, 509 (29 March 2012) doi:10.1038/483509a

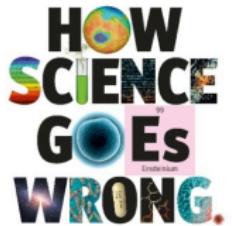
Published online: 28 March 2012

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Too many sloppy mistakes are creeping into scientific papers. Lab heads must look more rigorously at the data — and at themselves.

The Economist

Washington's lawyer scruples  
How to do a nuclear deal with Iran  
Investment tips from Nobel economists  
Junk bonds are back  
The meaning of Sezin Tendilur



# SCIENTIFIC MISCONDUCT ? WHAT ARE THE CONSEQUENCES ?

## The Duke University scandal with scientific misconduct on lung cancer

- *Nature Medicine* - 12, (2006) Genomic signatures to guide the use of **chemotherapeutics**, by Anil Potti and 16 other researchers from Duke and USF
- Major commercial labs licensed it and were about to start using it before two statisticians discovered and publicized its faults

Dr. Baggerly and Dr. Coombes found errors almost immediately. Some seemed careless — moving a row or a column over by one in a giant spreadsheet — while others seemed inexplicable. The Duke team shrugged them off as “clerical errors.”

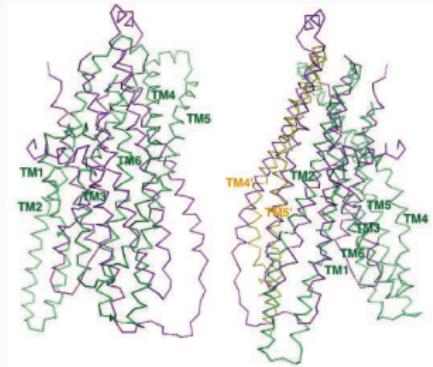
The Duke researchers continued to publish papers on their genomic signatures in prestigious journals. Meanwhile, they started three trials using the work to decide which drugs to give patients.

- Retractions: January 2011. Ten papers that Potti coauthored in prestigious journals were retracted for varying reasons

## Bad science is deleterious

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

# UNFORTUNATE MISTAKES



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 computational biology

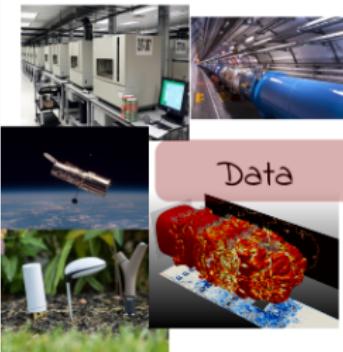
# DIFFERENT REPRODUCIBILITY CONCERNS

**Social Sciences, Oncology, ...** methodology, statistics

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

**Computational fluid dynamics** numerical issues

## Authors



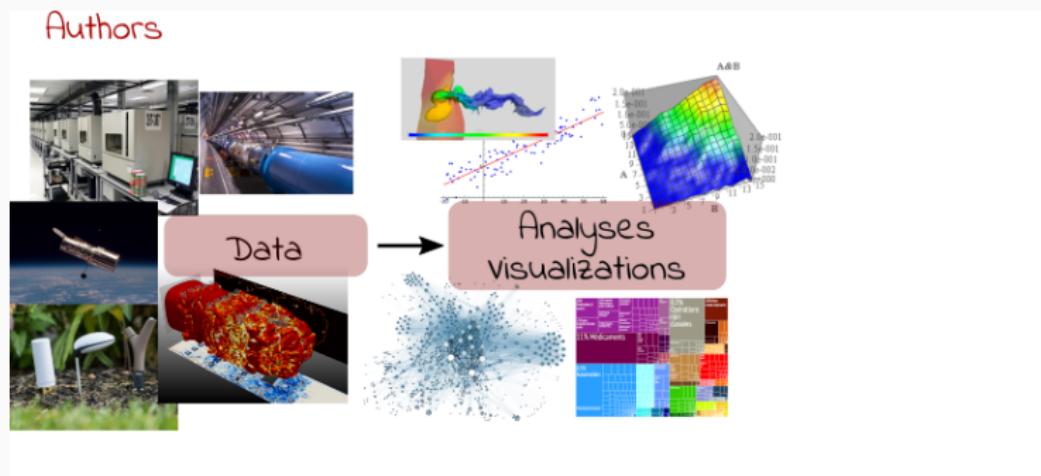
Data

# DIFFERENT REPRODUCIBILITY CONCERN

Social Sciences, Oncology, ... methodology, statistics

Genomics software engineering, computational reproducibility, provenance, ...

Computational fluid dynamics numerical issues

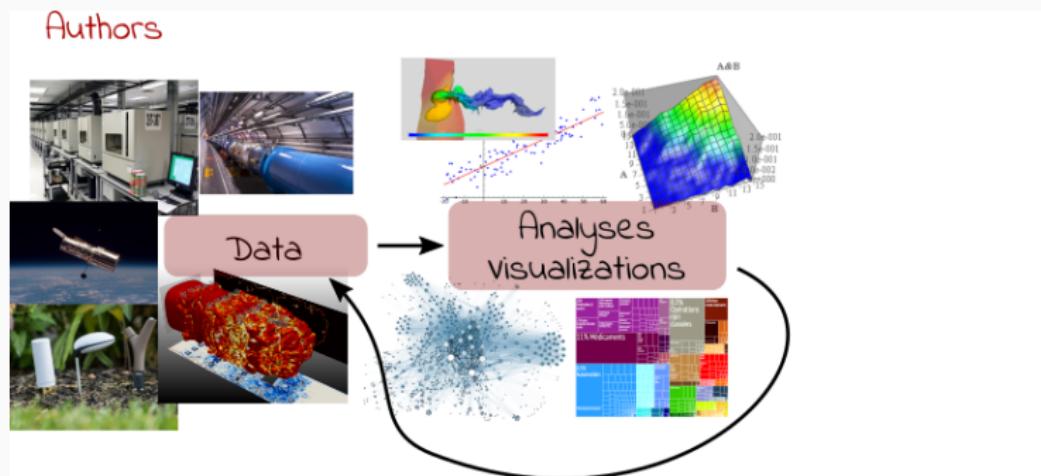


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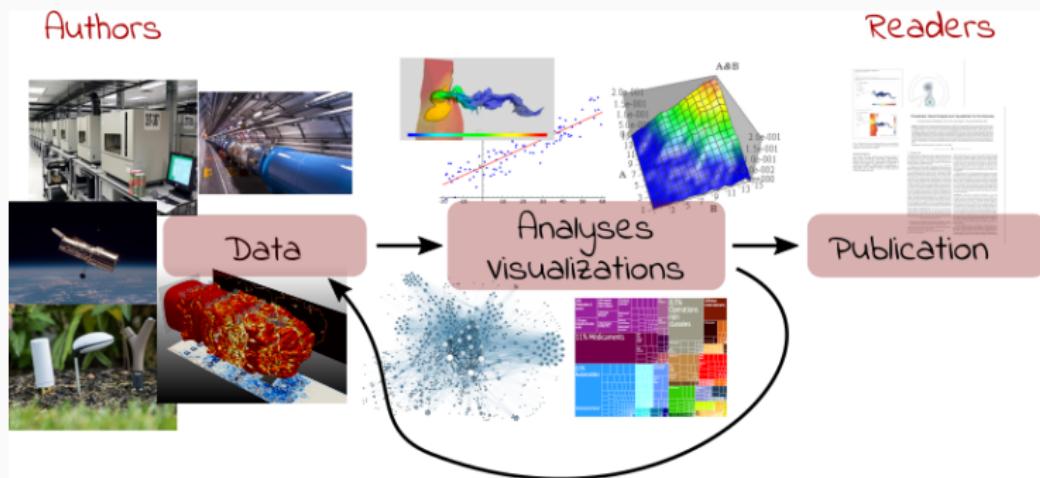


# DIFFERENT REPRODUCIBILITY CONCERN

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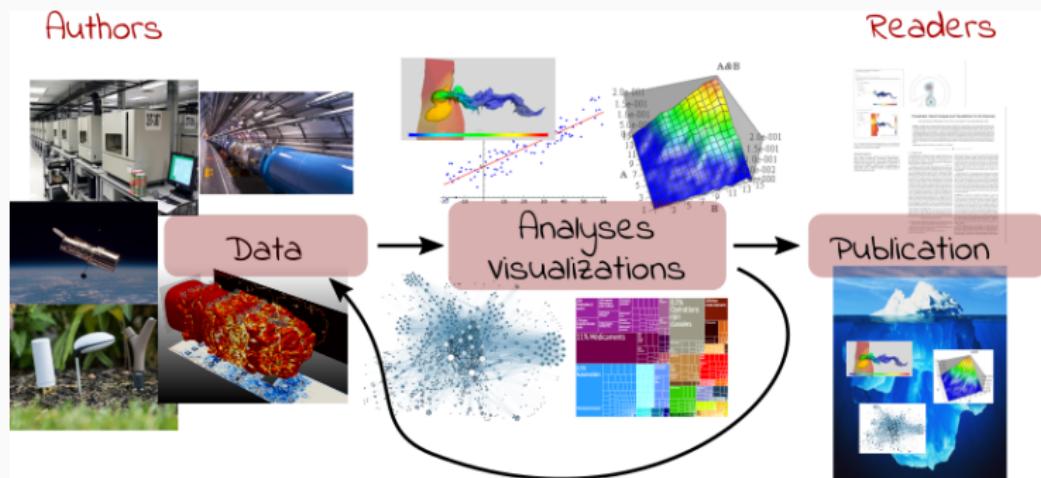


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Computational fluid dynamics numerical issues

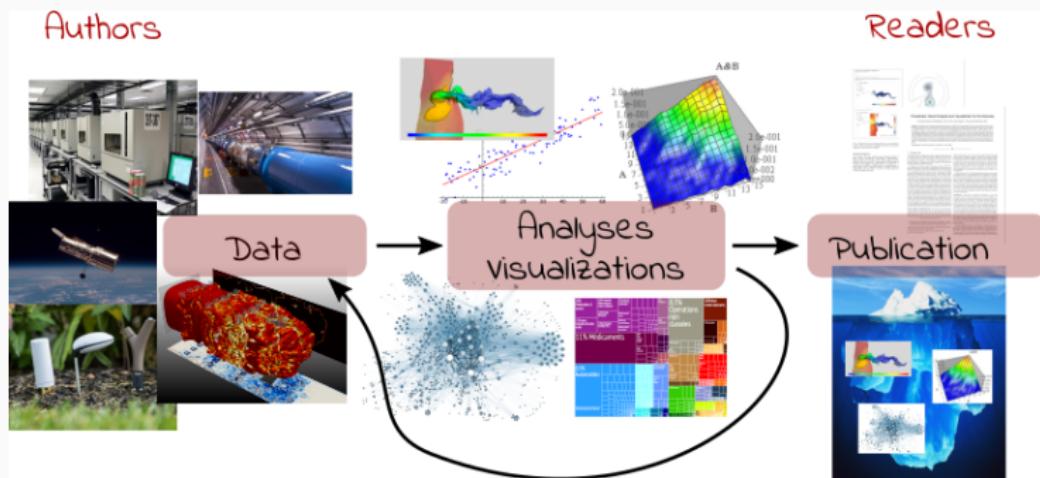


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Social Sciences, Oncology, ... methodology, statistics

Genomics software engineering, computational reproducibility, provenance, ...

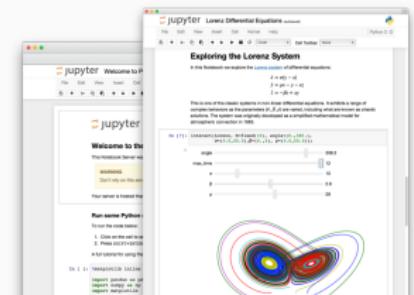
Computational fluid dynamics numerical issues



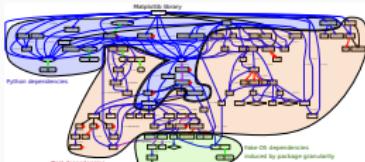
Reproducible Research = Bridging the Gap by working Transparently

# EXISTING TOOLS, EMERGING STANDARDS

## Notebooks and workflows



## Software environments



## Sharing platforms



# CHANGING RESEARCH PRACTICES

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



- Book on RR *Vers une recherche  
reproductible: Faire évoluer ses pratiques*
- MOOC on RR (3rd edition Feb. 2020)
- A new "Advanced RR" MOOC (Oct. 2020)
  - Software environment control (Docker)
  - Scientific workflow (snakemake)
  - Managing data (HDF5, archiving)

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

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

# CHANGING PUBLISHING PRACTICES

## Artifact evaluation and ACM badges



## Major conferences

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



Joelle Pineau @ NeurIPS'18

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

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

# REPRODUCIBLE RESEARCH = RIGOR AND TRANSPARENCY

To err is human.

Good research requires time and resources

1. **Train yourself and your students:** RR, statistics, experiments
  - Beware of checklists and norms
  - Understand what's at stake
2. **Change the norm:** make publication practices evolve
3. **Incentive:** consider RR/open science when hiring/promoting



# SOME ADVERTISING

**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, ResScience, Comité pour la Science Ouverte,  
UMI32 Bordeaux & Mission de la pédagogie et du numérique pour l'enseignement supérieur

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

# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Un document computationnel

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

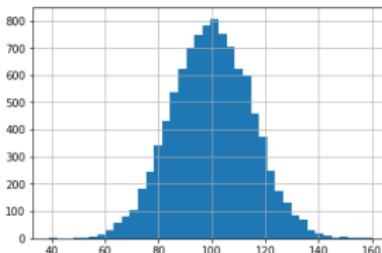
3.141592653589793

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 window titled "example\_ip" (modified). It contains three code cells:

- In [1]:**

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

 Output: 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 obtient d'abord 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
```

 Output: 3.14371986944998765
- 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()
```

 Output: A histogram showing a normal distribution centered at 100.

Document final

## Un document computationnel

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

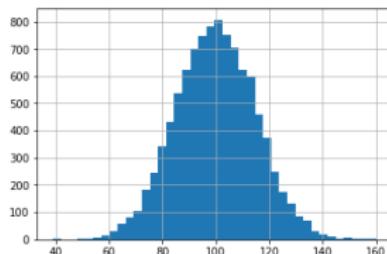
3.141592653589793

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
```

3.14371986944998765

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... ☺).



# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

Document initial dans son environnement

Jupyter example\_pl (modified)

# Un document computationnel

Mais 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](#) ([https://fr.wikipedia.org/wiki/Aiguille\\_de\\_Buffon](https://fr.wikipedia.org/wiki/Aiguille_de_Buffon)), on obtient aussi 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=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
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()
```

800  
700  
600  
500  
400  
300  
200  
100  
0

40 60 80 100 120 140 160

Document final

## Un document computationnel

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

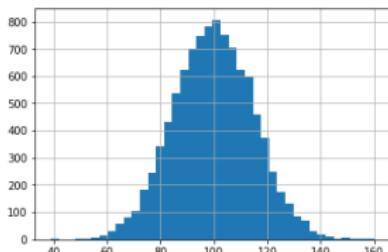
3.141592653589793

Mais calculé avec la [méthode des aiguilles de Buffon](#), on obtient 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=np.pi/2)
2/(sum((x+np.sin(theta))>1))/N
```

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... ☺).



# 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 Buffon's needle method.
- In [2]:** Calculates the area under a sine wave from 0 to pi/2 using the Monte Carlo method, resulting in 3.1437198694098765.
- In [3]:** Plots a histogram of 100 random numbers between 0 and 100, showing a bell-shaped distribution centered around 50.

Annotations with red arrows point from the text "Code" in the first section to the code blocks in the notebook, and from the text "Document initial dans son environnement" to the top of the screenshot.

Document final

## Un document computationnel

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

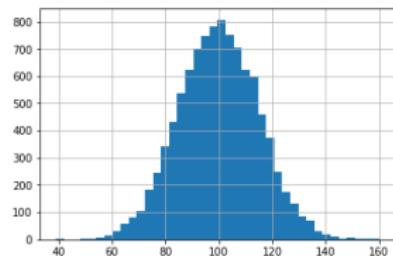
3.141592653589793

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

# Un document computationnel

```
In [1]:  
from math import *  
print(pi)  
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]: 3,143719869498765
```

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

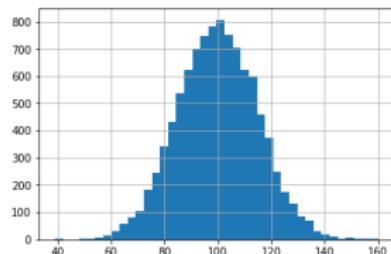
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```
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x = np.random.uniform(size=N, low=0, high=1)  
theta = np.random.uniform(size=N, low=0, high=pi/2)  
2/(sum((x+np.sin(theta))>1))/N
```

3.143719869498765

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 with the Buffon needle method.
- In [2]:** Generates random points (x, theta) and calculates an approximation of pi based on the ratio of points where x <= mu.
- In [3]:** Plots a histogram of x values, showing a bell-shaped distribution centered around 100.

Document final

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

3.141592653589793

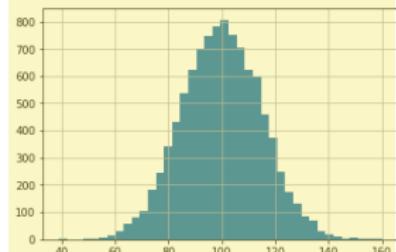
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```
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x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1))/N
```

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 three code cells:

- In [1]:** Prints the value of pi (3.141592653589793) and includes a note about calculating pi with the Buffon's needle method.
- In [2]:** Generates random points (x, theta) and calculates an approximation of pi based on the ratio of points where x <= sin(theta).
- In [3]:** Plots a histogram of x values, showing a bell-shaped distribution centered around 100.



Document final

## Un document computationnel

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

3.141592653589793

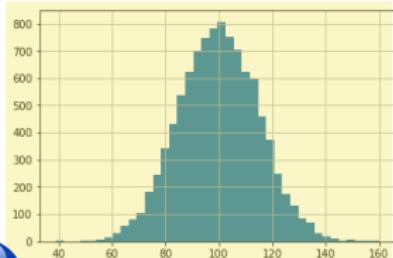
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```
import numpy as np
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1))/N
```

3.1437198694098765

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 2: FIGHTING SOFTWARE ENVIRONMENTS NIGHTMARE

What is hiding behind a simple

```
1 import matplotlib
```

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

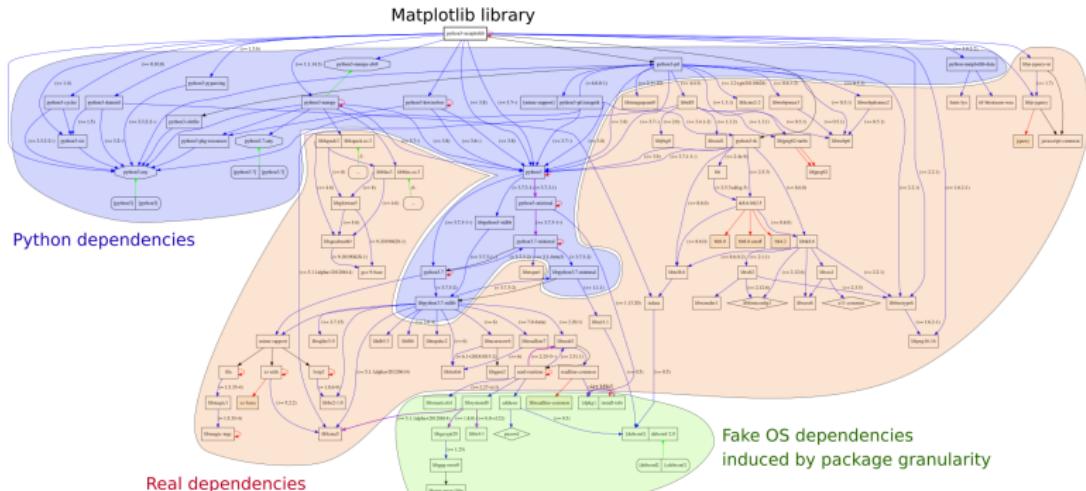
## TOOL 2: FIGHTING SOFTWARE ENVIRONMENTS NIGHTMARE

## What is hiding behind a simple

1

```
import matplotlib
```

Package: python3-matplotlib



## TOOL 2: FIGHTING SOFTWARE ENVIRONMENTS NIGHTMARE

Python and its rapidly evolving environment

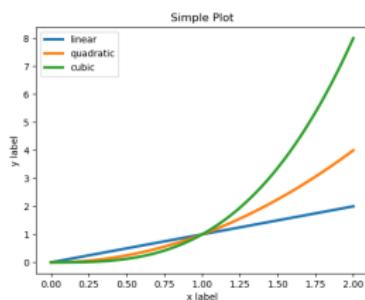
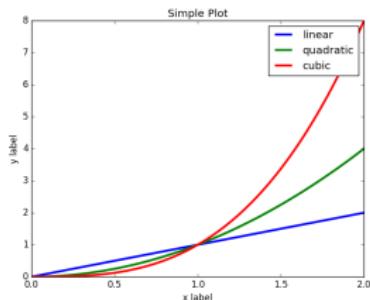
```
1 python2 -c "print(10/3)"  
2 python3 -c "print(10/3)"
```

```
3  
3.333333333333335
```

## TOOL 2: FIGHTING SOFTWARE ENVIRONMENTS NIGHTMARE

Python and its rapidly evolving environment

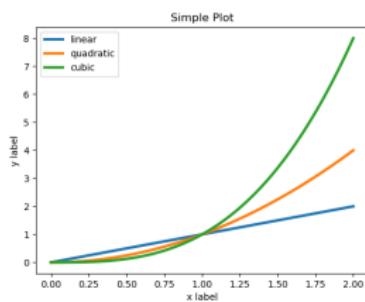
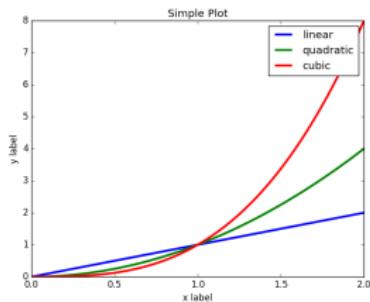
```
1 python2 -c "print(10/3)"  
2 python3 -c "print(10/3)"
```



## TOOL 2: FIGHTING SOFTWARE ENVIRONMENTS NIGHTMARE

Python and its rapidly evolving environment

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

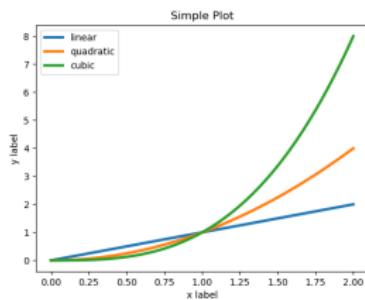
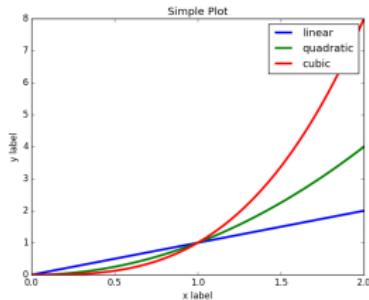


Cortical Thickness Measurements (PLOS ONE, June 2012): *FreeSurfer: differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

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## TOOL 3: FIGHTING INFORMATION LOSS WITH ARCHIVES

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

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*half life ranged from 2.2 years in EMHJ to 5.3 years in BMJ*

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