

# REPRODUCIBLE RESEARCH AND BENCHMARKING

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Arnaud Legrand



Inria foresight seminar

Optimization, Machine Learning and Statistical Methods

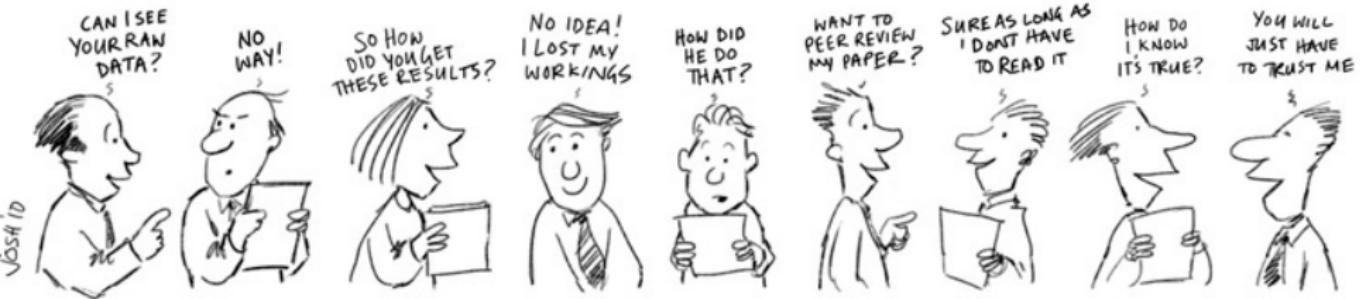
October 2023



## SCIENTIFIC CONSENSUS VS. DEMOCRACY AND FREEDOM OF SPEECH



# NO TRANSPARENCY NO CONSENSUS



# REPRODUCIBLE RESEARCH ~ 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



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NO CONSENSUS**



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

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- CELESTE: bound false positive error rate while maximizing power, robustness
- MODAL: ML performance assessment (~~misleading conclusions~~)

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- **SCOOL**: *Software development is not in our genes in Scool and we did not see how we might contribute in a useful manner until recently*
  - **rlberry**: *a Reinforcement Learning library for Research and Education Reaction of PhD students to have an open-source library with state-of-the-art implementations of RL algorithms*

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  - **rlberry**: *a Reinforcement Learning library for Research and Education*  
*Reaction of PhD students to have an open-source library with state-of-the-art implementations of RL algorithms*
- **SIERRA**: *potentially long, non-intuitive, and technical, proofs*
  - ↗ computer-aided proofs, techniques gathered in a software package, **PEPit**, for helping *producing and reproducing convergence proofs*

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  - **POT** (optimal transport): *implementations of more than 40 research papers providing new solvers*
- **RANDOPT, TAU, OCKHAM**: **benchmarking frameworks** and **organizing challenges**
  - Target = **Fair comparison** and **Animation of the community**
  - **COCO**, **BenchOpt**, **Codalab**

# DIFFERENT REPRODUCIBILITY CONCERNS IN MODERN SCIENCE

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

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**Computational fluid dynamics** numerical issues

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

## Authors



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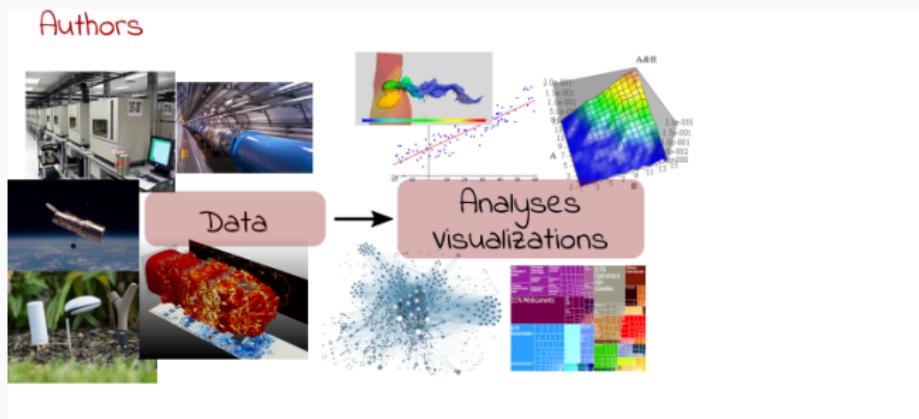
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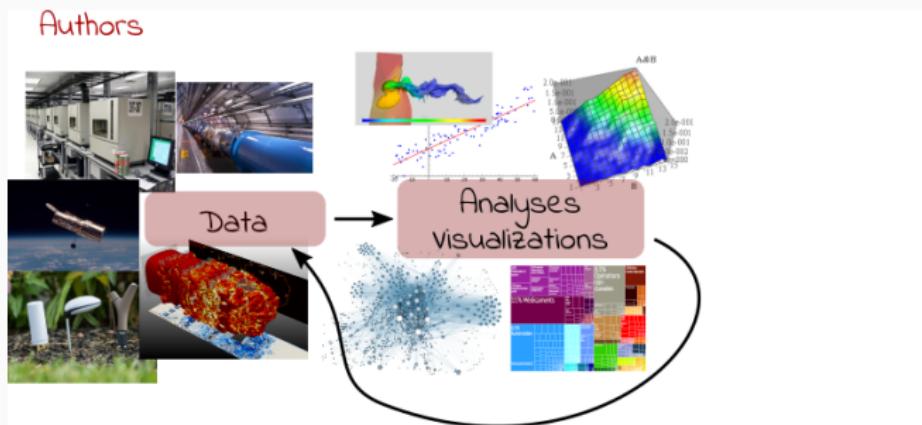
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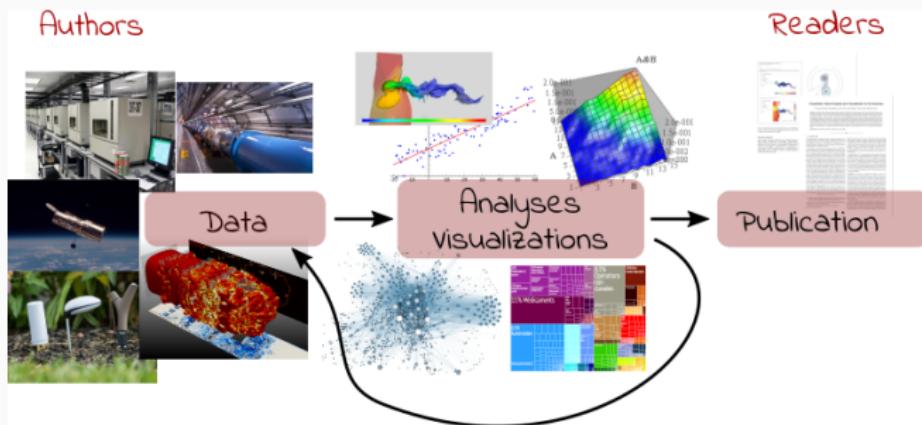
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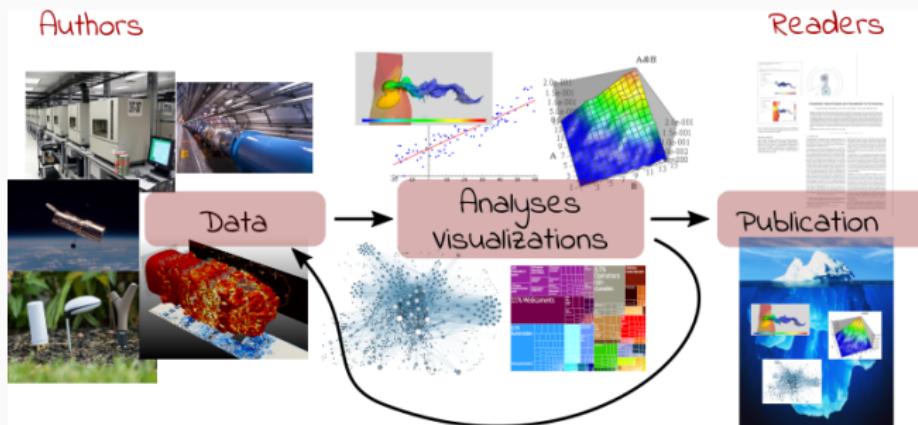
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Reproducible Research = Bridging the Gap by working Transparently

# REPRODUCIBILITY (GLOSSARY MAY VARY)

Many (conflicting) **definitions** (*replicability, repeatability, reproducibility, corroboration*)  
(*new data, same person, independant 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	same 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

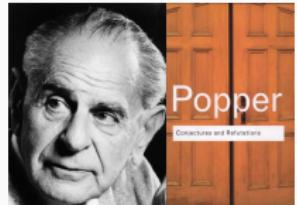
<sup>2</sup>Independently from (random) sampling variability (fight bias)

<sup>3</sup>Bitwise

# REPRODUCIBILITY OF EXPERIMENTAL RESULTS: THE HALLMARK OF SCIENCE

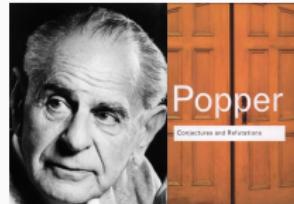
1934: Karl Popper puts the notions of **falsifiability** and **crucial experiment** as the **hallmark of science**

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



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

# 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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*Today the computer is just as important a tool for chemists as the test tube. Simulations are so realistic that they predict the outcome of traditional experiments...*

– Nobel Comity (Chemistry), 2013

But, scientific practices have greatly evolved, in particular since we rely on computers, statistics, machine learning, complex black boxes, ...

REPRODUCIBILITY: BOTH AN  
INTERNAL AND EXTERNAL PROBLEM  
FOR CS/ML/...

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# COMPUTERS...

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

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



– Ben Marwick,  
The conversation, 2015

**Point-and-click** procedures are rampant but they hinder reproducibility.

**Spreadsheets** are generalized and intensively used in biology:

- **Membrane-Associated Ring Finger (C3HC4) 1,**  
**E3 Ubiquitin Protein Ligase** → **MARCH1** → 2016-03-01 →  
1456786800
- **2310009E13** → 2.31E+19

And more recently, we had the **COVID tracing failure**.



## Machine Learning: Trouble at the lab, The Economist 2013

*According to some estimates, three-quarters of published scientific papers in the field of machine learning are bunk because of this "overfitting".*

– Alex "Sandy" Pentland

## The Reproducibility Crisis in ML-based science (Princeton workshop 2022)

*Reproducibility failures in ML-based science are systemic. We found 20 reviews across 17 scientific fields (medicine, neuroimaging, autism diagnosis, genomics, computer security, ...) that find errors in a total of 329 papers that use ML-based science and in some cases leading to wildly overoptimistic conclusion. [...] complex ML models don't perform substantively better than decades-old LR models.*

*Data leakage:* spurious relationship between the independent variables and the target variable that arises as an artifact of the data collection, sampling, or pre-processing strategy.

– S. Kapoor and A. Narayanan

## THIS IS ABOUT COMPUTATIONAL SCIENCE. SHOULD MATHEMATICIANS CARE?

Computer Science is young and inherits from Mathematics, Engineering,  
Linguistic, Nat. Sciences, ...

Purely theoretical scientists whose practice is close to mathematics may not be concerned (can't publish a math article without releasing the proofs).

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Yet, incoherencies are common, especially in a fast moving field:

- E.g., definitions/concepts in book/article A and B are *slightly different* and the resulting theorems cannot be mixed
- Have a look at Vladimir Voevodsky's talk in 2014 at Princeton 😊
  - ↪ computer-aided proofs in SIERRA
- ERC Nano bubbles: how, when and why does science fail to correct itself?

Flagging incorrect nucleotide sequence reagents in biomedical papers:

To what extent does the leading publication format impede automatic error detection?

(Labbe et al., 2020)

## EMERGING TOOLS AND PRACTICES

---

# MAIN CHALLENGES

```
1 my_code --cfg=magical_param:0.94572 *.dat --output foo.csv
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## Tracking code version

- `my_code` is revision `21b95ecfa0911d6ca87668482b11ab9498edd8f3`

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## Handle complex sequences and reuse results (leverage supercomputers)

# TOOL 1: COMPUTATIONAL NOTEBOOKS/LITTERATE PROGRAMMING

## Un document computationnel

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

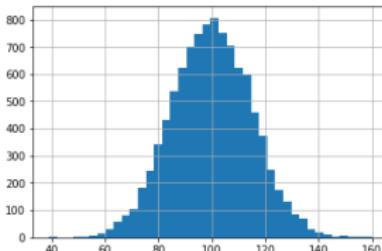
3.141592653589793

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
```

A note below it says: "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 l'air comme approximation :".
- In [2]:** A code cell containing:

```
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
```

A note below it says: "On peut inclure des formules mathématiques comme  $\sqrt{2\pi}/(\exp(-x^2/2))$  et des dessins qui n'ont rien à voir avec  $\pi$ , avec `!jupyter` (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()
```

A histogram plot showing a bell-shaped curve centered at approximately 100.

Document final

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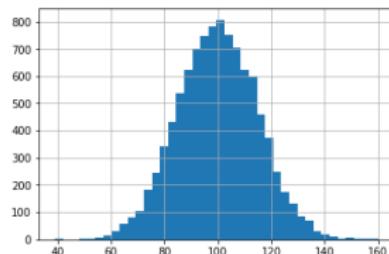
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The screenshot shows a Jupyter Notebook interface with three code cells:

- In [1]:** A text cell containing "# Un document computationnel". Below it, a code cell with the Python code: 

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 and its 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 une approximation :".
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```

 and its output: "Out[2]: 3.1437198694998765". Below it, a text cell with the 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... ☺)".
- In [3]:** A code cell with the Python code: 

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mu, sigma = 100, 15  
x = mu + sigma*np.random.randn(10000)  
  
plt.hist(x,40)  
plt.grid(True)  
plt.show()
```

 and its output: a histogram of a normal distribution centered at 100.

Document final

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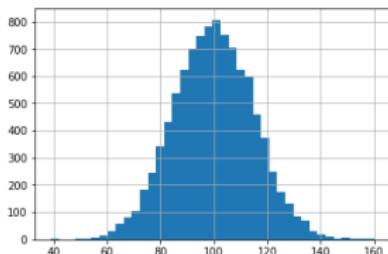
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A screenshot of a Jupyter Notebook interface. The title bar says "jupyter example\_pi". The main area shows two code cells:

In [1]:

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from math import *
print(pi)
3,141592653589793
```

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
```

In [3]:

```
%matplotlib inline
import matplotlib.pyplot as plt
mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)
plt.hist(x,60)
plt.grid(True)
plt.show()
```

The output of cell 3 is a histogram of 10,000 random numbers drawn from a normal distribution centered at 100 with standard deviation 15. The x-axis ranges from 40 to 160, and the y-axis ranges from 0 to 800. The histogram shows a bell-shaped curve.

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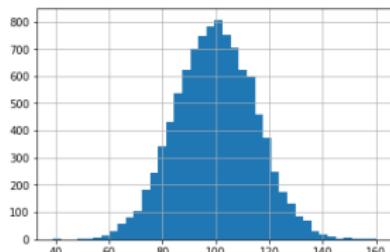
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import matplotlib.pyplot as plt  
  
mu, sigma = 100, 15  
x = mu + sigma*np.random.randn(10000)  
  
plt.hist(x, 99)  
plt.grid(True)  
plt.show()
```

Résultats

Document final

## Un document computationnel

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

3.141592653589793

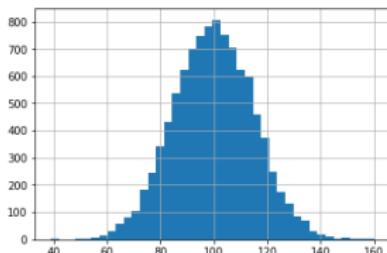
Mais calculé avec la méthode des aiguilles de Buffon, on obtiendrait comme approximation :

```
import numpy as np  
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 with the Buffon needle method.
- In [2]:** Generates random points (x, theta) and calculates an approximation of pi based on the ratio of points falling within a circle of radius 1 centered at (mu, 0).
- 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

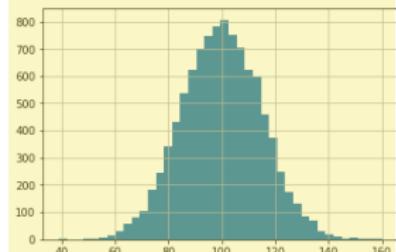
Mais calculé avec la **méthode des aiguilles de Buffon**, on obtiendrait comme approximation :

```
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]:** `from math import *  
print(pi)` Output: 3,141592653589793
- 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: 3,1437198694098765
- In [3]:** `import matplotlib.pyplot as plt  
mu, sigma = 100, 15  
x = mu + sigma*np.random.randn(10000)  
plt.hist(x, 100)  
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

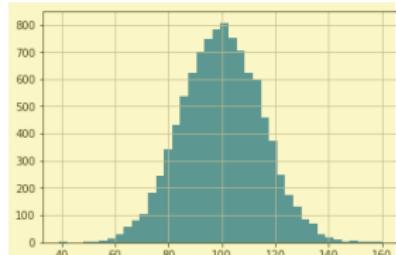
Mais calculé avec la **méthode des aiguilles de Buffon**, on obtiendrait comme approximation :

```
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
```

3.1437198694098765

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... ☺).



# TRACKING THE EXPLORATION PROCESS WITH A NOTEBOOK

The *REPL* (Read–eval–print loop) vs. *Notebook* vs *IDE* debate

- In the beginning was the Mathematica (1988) and the Maple (1989) notebooks, which allow to tell a story ([literate programming](#))

# TRACKING THE EXPLORATION PROCESS WITH A NOTEBOOK

The *REPL* (Read–eval–print loop) vs. Notebook vs *IDE* debate

- In the beginning was the Mathematica (1988) and the Maple (1989) notebooks, which allow to tell a story (*literate programming*)
- Then IJulia, IPython, and IR merged into the Jupyter notebook 😊
  - The coolest kid on the block without ~~IDE/Structure~~,  
~~Interactive collaboration/Versioning~~,  
~~Software Environment Control~~,  
~~Easy setup and use of Computing resources~~ !!! 😞

# TRACKING THE EXPLORATION PROCESS WITH A NOTEBOOK

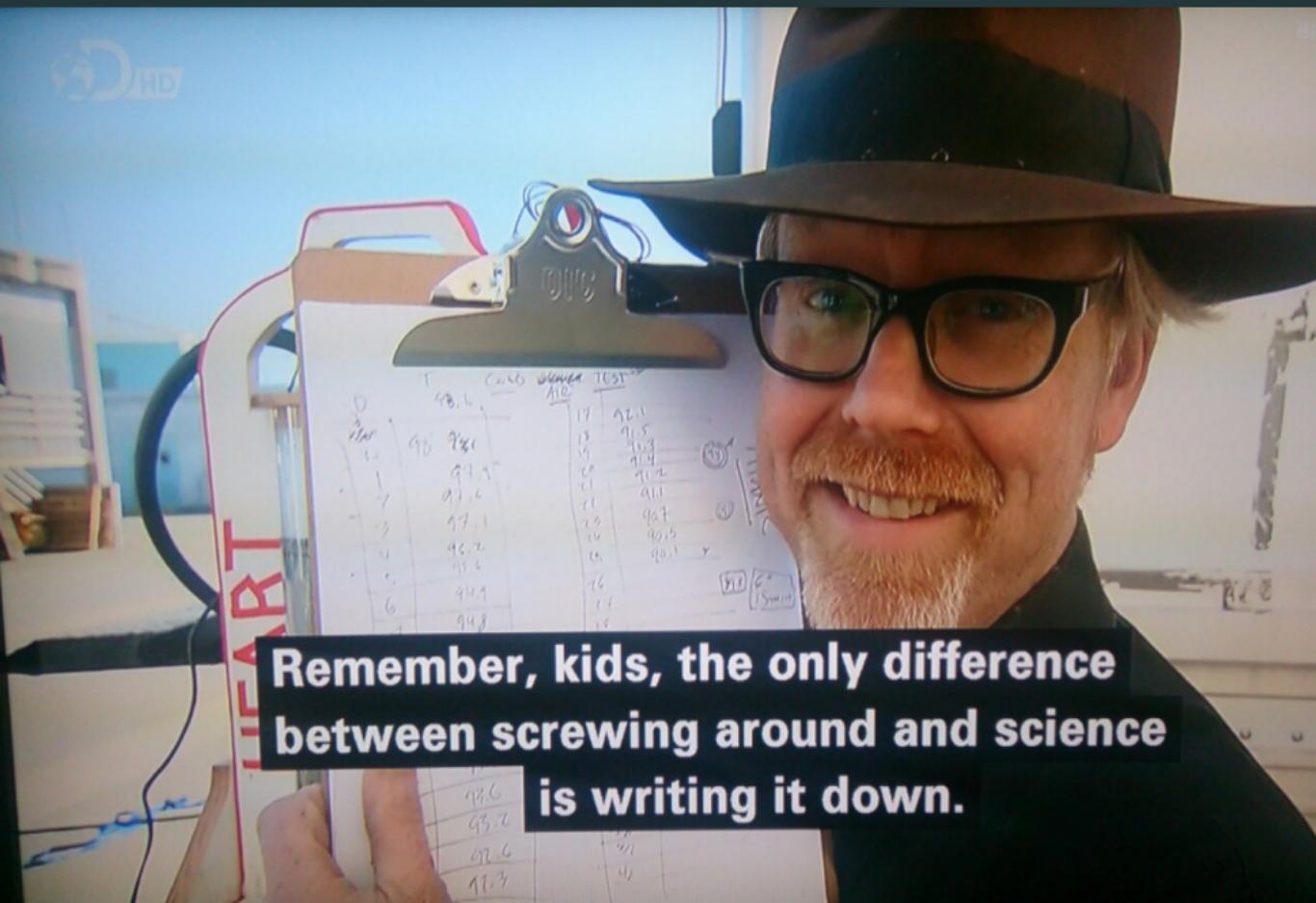
The *REPL* (Read–eval–print loop) vs. Notebook vs *IDE* debate

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- Then JJulia, IPython, and IR merged into the Jupyter notebook 😊
  - The coolest kid on the block without ~~IDE/Structure~~,  
~~Interactive collaboration/Versioning~~,  
~~Software Environment Control~~,  
~~Easy setup and use of Computing resources~~ !!! 😞

Now we have:

- JupyterLab, Binder, JupyterHub
  - Guix-Jupyter
- IDE: Rstudio (not just R), Emacs, VSstudio (Jupyter~backend)
- CodeOcean *showroom, interactive*
- CoCalc/SAGE notebooks, Kaggle, Google Colab, DeepNote  
*real-time, versioning, custom environment*
- fast.ai/nbdev  
*merge conflict, module export, test*
- Beaker, Count 😕 ???

## 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

The screenshot shows a Jupyter Notebook interface with the title bar "jupyter example\_pi.ipynb". The notebook contains several cells:

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

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

A note below it says: "Mais calculé avec la `__method__` des (ajoutées de Buffet) `__str__` et `__repr__` de `math`, on obtientrait comme approximation..."
- In [2]:** A code cell containing:

```
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)
((1/(n*theta)) * np.sin(theta)) > 1/N
```

Output: 0.1437198684495075
- In [3]:** A code cell containing:

```
%matplotlib inline
import matplotlib.pyplot as plt
N = 1000000
x = np.random.uniform(0, high=1)
y = np.sin(np.pi*x)
plt.hist(x,y)
plt.show()
```

Output: A histogram showing a bell-shaped curve centered at 0.5, with the x-axis ranging from 0 to 1 and the y-axis ranging from 0 to 800.

# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

jupyter analyse-syndrome-grippal Last Checkpoint 20 minutes ago (autosaved)

File Edit View Insert Cell Kernel Help Hide Code Export to HTML

In [1]: `#!/usr/bin/python3  
# Analyse du syndrome grippal au CHU de Toulouse`

Les données de l'Institut de Santé Publique sont disponibles à ce lien : <https://biostats.maths.tufts.edu>. Nous les disposons sous forme d'un fichier zip nommé 'syndrome\_grippal.zip'. Pour décompresser le fichier ZIP et l'ouvrir dans un explorateur de fichiers faites faire une double clic sur le zip pour ouvrir le dossier contenant les données.

Voici quelques lignes de code pour charger les données et les visualiser :

```
import pandas as pd
df = pd.read_csv('syndrome_grippal.csv')
```

In [2]: `# Afficher les 5 premières lignes du DataFrame`

```
df.head()
```

Out[2]:

date	age	genre	nb_victimes	nb_victimes_95ci_low	nb_victimes_95ci_high	nb_victimes_psi_low	nb_victimes_psi_high
2008-01-01	0-4	F	116	106	126	101	131
2008-01-01	0-4	M	116	106	126	101	131
2008-01-01	5-19	F	116	106	126	101	131
2008-01-01	5-19	M	116	106	126	101	131

On peut voir que les victimes sont principalement des enfants de moins de 20 ans, avec un peu plus de 100 victimes par jour dans la population française.

In [3]: `# Calculer la moyenne des victimes par jour`

```
df['nb_victimes'].mean()
```

Out[3]: 289.285

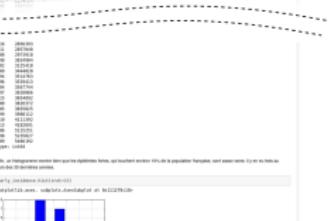
Environ 289 personnes sont malades par jour dans la population française, soit environ 0.1% de la population française, soit environ 100 000 personnes.

In [4]: `# Importer les bibliothèques nécessaires`

```
#!/usr/bin/python3  
# Analyse du syndrome grippal au CHU de Toulouse
```

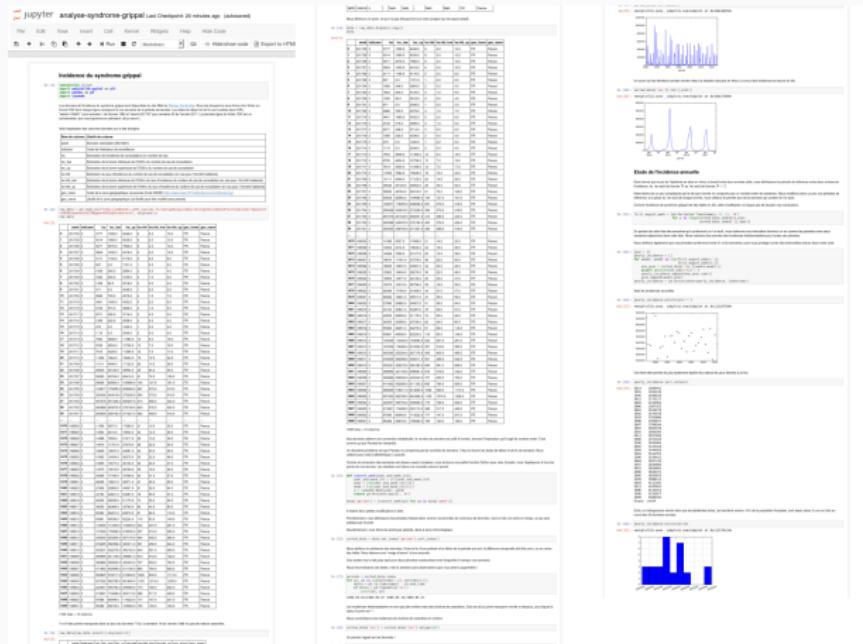
In [5]: `#!/usr/bin/python3  
# Analyse du syndrome grippal au CHU de Toulouse`

Figure showing the daily average number of victims:



# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code



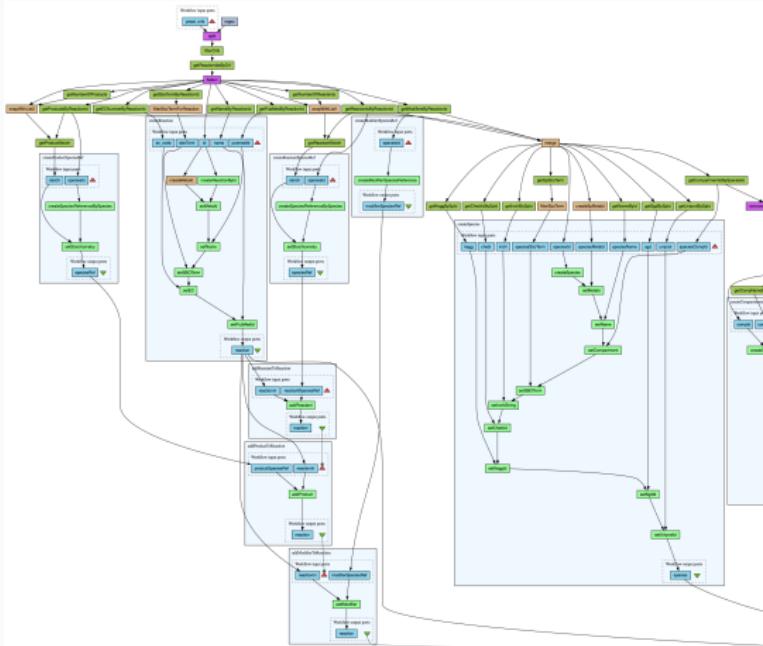
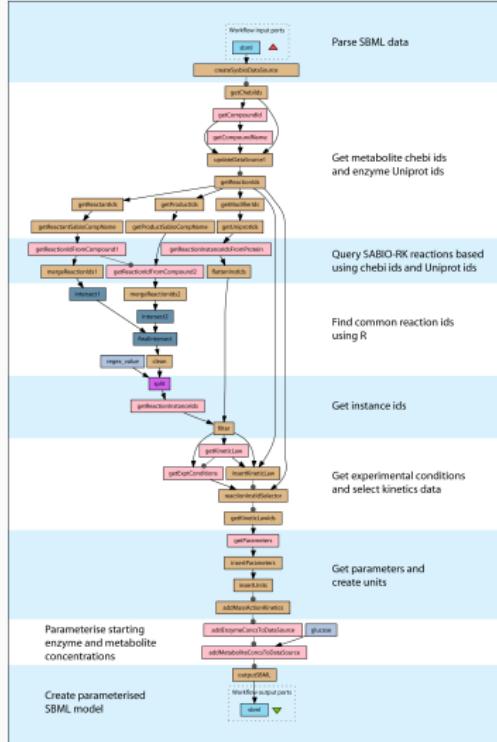
# TOOL 1 TER: WORKFLOWS

Notebooks are no panacea and do not help developing clean code

The image displays a 4x3 grid of Jupyter Notebook screenshots, each showing a different step or aspect of a data science workflow. The notebooks include code snippets, explanatory text, and visualizations such as scatter plots and heatmaps.

- Cell 1: Estimating Color Names by Web Image**  
This cell shows code for extracting colors from a web image. It includes a screenshot of the image and a color palette visualization.
- Cell 2: Dimensionality reduction**  
This cell discusses dimensionality reduction, specifically PCA, and includes a snippet of Python code.
- Cell 3: Dimensionality reduction**  
This cell continues the discussion on dimensionality reduction, mentioning t-SNE and PCA.
- Cell 4: Dimensionality reduction**  
This cell provides a detailed explanation of t-SNE, including its mathematical formula and parameters.
- Cell 5: Dimensionality reduction**  
This cell shows a snippet of Python code for dimensionality reduction.
- Cell 6: Dimensionality reduction**  
This cell continues the discussion on dimensionality reduction, mentioning t-SNE and PCA.
- Cell 7: Dimensionality reduction**  
This cell provides a detailed explanation of t-SNE, including its mathematical formula and parameters.
- Cell 8: Dimensionality reduction**  
This cell shows a snippet of Python code for dimensionality reduction.
- Cell 9: Dimensionality reduction**  
This cell continues the discussion on dimensionality reduction, mentioning t-SNE and PCA.
- Cell 10: Dimensionality reduction**  
This cell provides a detailed explanation of t-SNE, including its mathematical formula and parameters.
- Cell 11: Dimensionality reduction**  
This cell shows a snippet of Python code for dimensionality reduction.
- Cell 12: Dimensionality reduction**  
This cell continues the discussion on dimensionality reduction, mentioning t-SNE and PCA.

# 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
    - SoS Polyglot Notebook/Workflow System

## Examples:

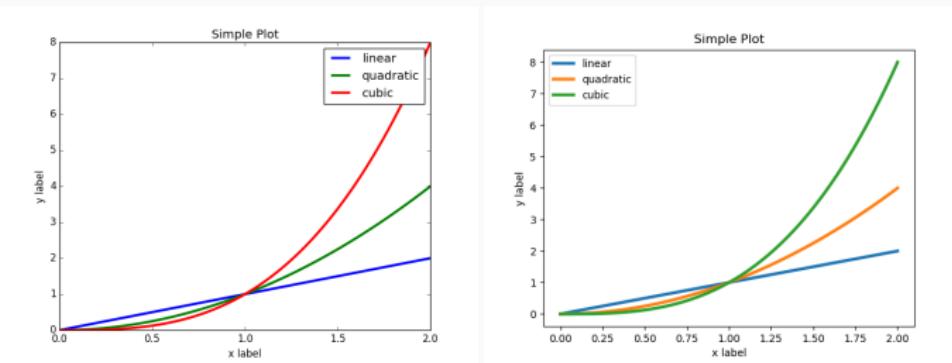
- Galaxy, Kepler, Taverna, Pegasus, Collective Knowledge, VisTrails
- Light-weight: **make**, dask, drake, swift, **snakemake**, ...

## SOFTWARE DEPENDENCIES: HORROR STORIES

---

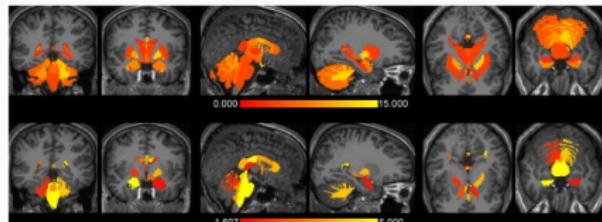
# SOFTWARE DEPENDENCIES: HORROR STORIES

- 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%)

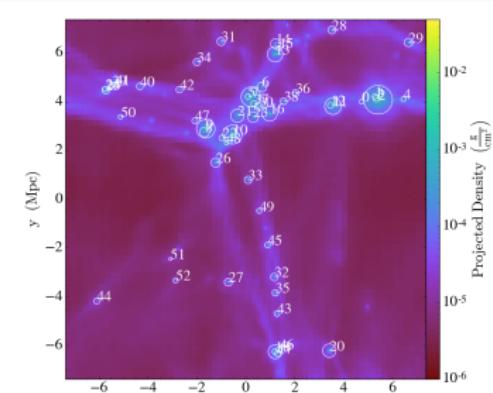
*About a factor two smaller differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

*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

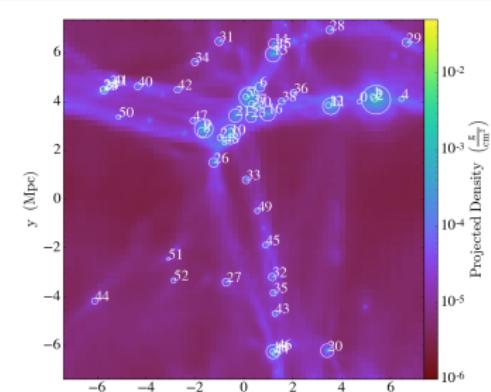


Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

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

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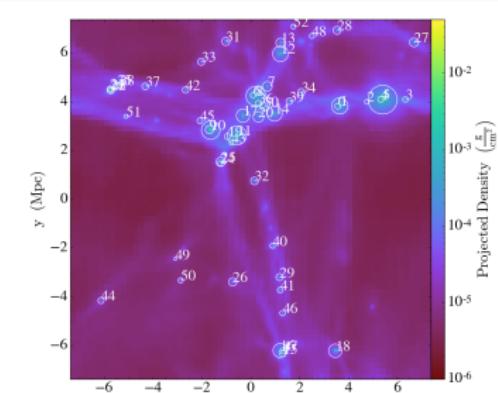


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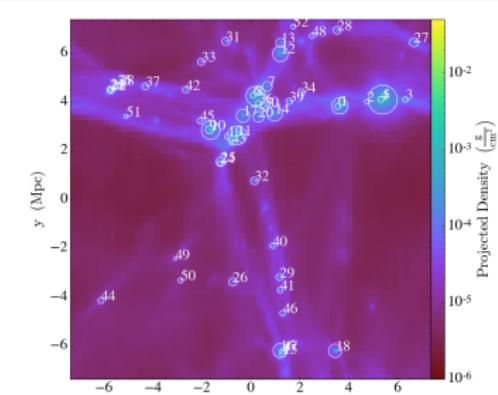


Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context (ResCuE-HPC, 2018)

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		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
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

## 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

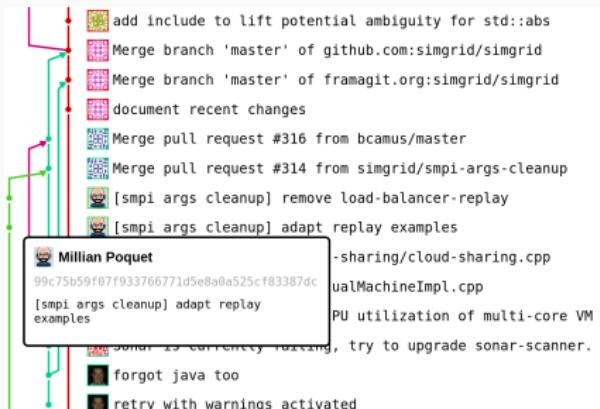
### Package managers (the ugly and the good)

- 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)

# TOOL 3: VERSION CONTROL AND FORGE

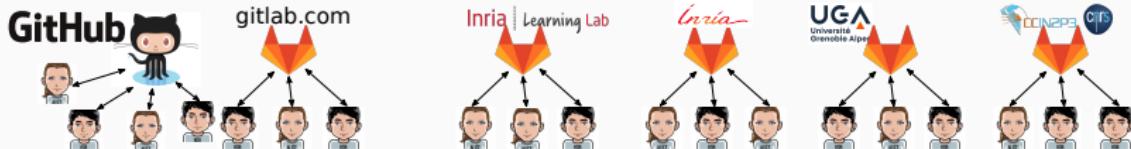
## Git = version control

- 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*
- 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

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Article archives



Data archives



Software Archive



Software Heritage

Collect/Preserve/Share

Separation between articles, code, and data is not so simple though

# TOOLS #4: MANAGING DATA, COMPUTATION, AND PROVENANCE

## Reinventing the square wheel

### Data Version Control with DVC

- **git annex** but special **.dvc** files with information about local/remote storage
- **snakemake** but Data Pipelines through a **dvc.yaml** task description
- A basic Workflow Management System with little support for running pipelines in parallel

### NetFlix (100,000+ jobs per day)

- Notebooks as functions with **papermill** ([Parameterized Notebooks](#))
- Run in **docker environments** using **MESON** (home made workflow orchestration/scheduler)
- Storage in S3, Dashboard like usage to generate daily reports

### DeepKit, PolyAxon, Pachyderm, Kono Lord, Have mercy!

- Versionned data without **git**, a centralized location (no conflict, allows removal,...)

Best tool I've seen so far: **git-annex** / **datalad**

## TREND #5: DELEGATING THE EXPERIMENT TO A THIRD PARTY

---

**CASCAD** certification agency for scientific code & data (for economists)

**Continuous Integration** Running experiments through CI

- Main concern: invisibility  $\rightsquigarrow$  crazy resource consumption

## CONCLUSION, CHALLENGES

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## CONCLUDING THOUGHTS

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► *The Structure of Scientific Revolutions*

– Thomas Kuhn

For 20 years, reproducibility issues have been a rampant problem, addressed by few isolated groups

## CONCLUDING THOUGHTS

---

### ► *The Structure of Scientific Revolutions*

– Thomas Kuhn

For 20 years, reproducibility issues have been a rampant problem, addressed by few isolated groups   Now, it is everywhere (ACM, ACM EIG, COARA, NIPS, ICML) and can be seen both as a **disruption**, a **threat**, or an **opportunity**, ...

- Benchmarking and challenges are one option
  - positive (federating the community)
  - negative (HPL, NAS PB)
  - sometimes limited gain
  - sometimes inadequate

# CONCLUDING THOUGHTS

---

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► *Anything goes*

– Paul Feyerabend

- Tension between original/groundbreaking research and strengthening foundations   Imposing RR globally and too soon can be deleterious

# CONCLUDING THOUGHTS

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- sometimes inadequate

## ► *Anything goes*

– Paul Feyerabend

- Tension between original/groundbreaking research and strengthening foundations   Imposing RR globally and too soon can be deleterious

It has become **insanely complex!** Level up with our PhD students.

- MOOC Reproducible Research: Methodological principles for a transparent science

- 3rd Edition: 2020 – 2024 (16,000+) | MOOC "Advanced RR" Feb. 2024

- Slow down and **keep things simple!**

*Monster models imply non-reproducible science, without even mentioning sustainability concerns and applicability concerns* – TAU 24/26

## THE SCIENCE IS CLEAR

Why are we  
ignoring it?

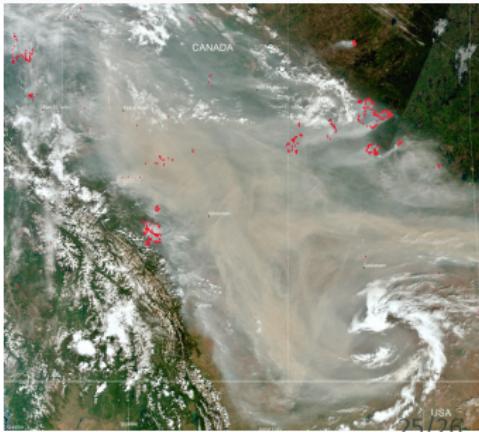
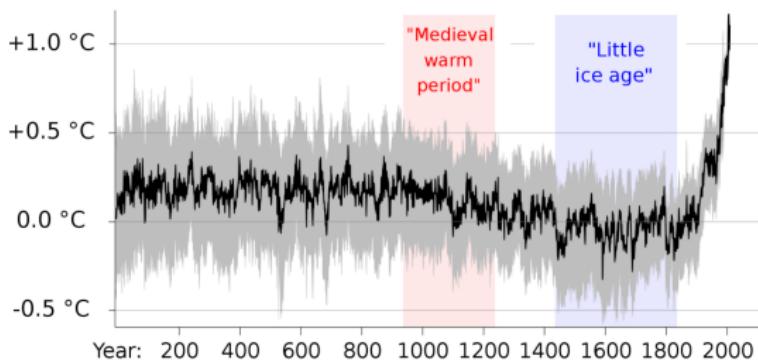
scientist rebellion

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

1. Global climate change is not a future problem



Global Average Temperature Change



# THE ELEPHANT IN THE ROOM: CLIMATE CHANGE

1/2

## THE SCIENCE IS CLEAR

Why are we  
ignoring it?

scientist rebellion

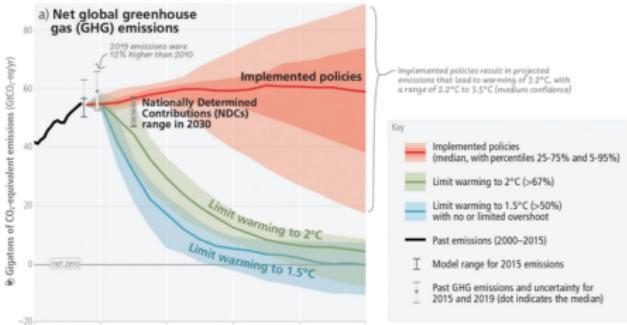


IPCC, IPBES, <https://climate.nasa.gov/>

1. Global climate change is **not** a future problem
2. It is **entirely** due to human activity

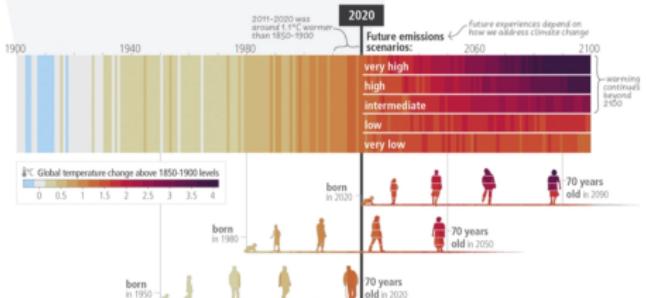
Limiting warming to **1.5°C** and **2°C** involves rapid, deep and in most cases immediate greenhouse gas emission reductions

Net zero CO<sub>2</sub> and net zero GHG emissions can be achieved through strong reductions across all sectors



Paris Agreement'15 ~ Net Zero by 2050

c) The extent to which current and future generations will experience a hotter and different world depends on choices now and in the near-term



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Latest IPCC report

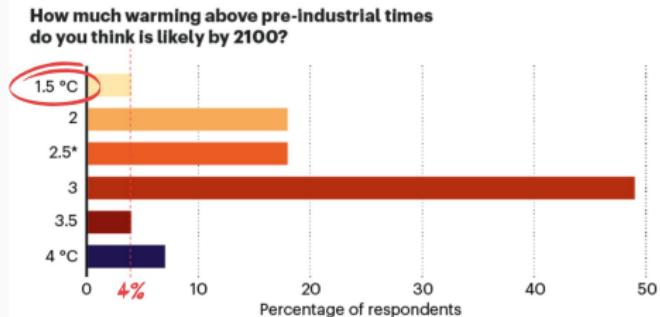
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1. Global climate change is **not** a future problem
2. It is **entirely** due to human activity
3. **9 out of 10 IPCC scientists believe overshoot is likely**



\*Includes 2 responses between 2.7 °C and 2.75 °C; 2.5 °C and 3.5 °C were write-in answers.

@nature

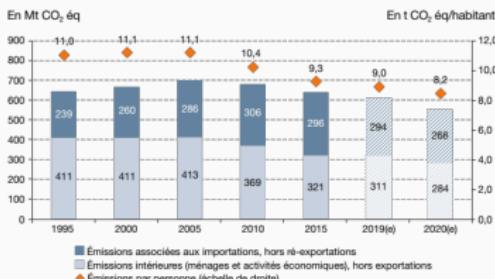
Nature survey, Nov. 2021

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# THE ELEPHANT IN THE ROOM: CLIMATE CHANGE

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

ÉVOLUTION DE L'EMPREINTE CARBONE DE LA FRANCE



Empreinte carbone moyenne en France  
10 tonnes de CO<sub>2</sub>e/an/pers.



÷2  
d'ici  
2030

<2t CO<sub>2</sub>e

Objectif d'ici 2050

- de 2 t de CO<sub>2</sub>e/an/pers.

+ Faire plus d'activités bas carbone !

Danser, chanter, jardiner, rêver, écire, lire, courir, randonner, planter des arbres, discuter, marcher en forêt, méditer, passer du temps avec ceux qu'on aime, lire...

Bref, inventer nos vies bas carbone désirables !

Par exemple :

0,5 t CO<sub>2</sub>e/Annee : à la maison, préférence à l'électrique et sans produits dérivés

0,5 t CO<sub>2</sub>e/Annee : faire une partie route (30%) de votre voiture (30%) de fabrication ancienne sur 30 ans, importer moins de 10% de vos denrées et faire moins de transports en commun.

0,5 t CO<sub>2</sub>e/Annee : faire moins de 40 km de trajet en voiture, faire diverses expérimenter des alternatives et interroger les acteurs, sobriété dans l'usage des denrées et services publics.

0,2 t CO<sub>2</sub>e/Annee : échafaudage sur un tapis de puzzle, 90% de nuit et d'un logement bien isolé

0,2 t CO<sub>2</sub>e/Annee : à la maison, passer à la chaleur ou solaire thermique.

0,2 t CO<sub>2</sub>e/Annee : faire évoluer les services publics : faire enseignement,

<https://www.nosviesbascarbonne.org/>

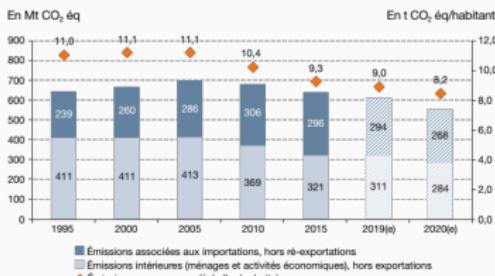
INVENTONS  
NOS VIES  
BAS CARBONE

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

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## French government response

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

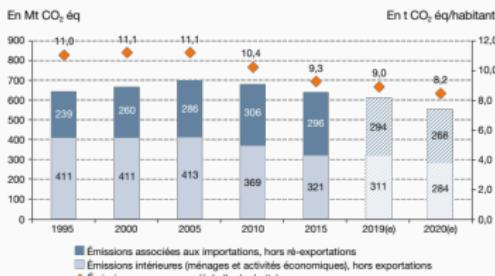


# THE ELEPHANT IN THE ROOM: CLIMATE CHANGE

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ÉVOLUTION DE L'EMPREINTE CARBONE DE LA FRANCE



(e) = estimations.

Note : l'empreinte carbone porte sur les trois principaux gaz à effet de serre (CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O). En 2021, la méthodologie a été ajustée afin de mieux tenir compte de l'évolution des coûts du pétrole brut, du gaz et du charbon. L'empreinte de la séries a ainsi été révisée, l'essentiel des ajustements portant sur les émissions importées de CH<sub>4</sub>.

Champ : périmètre Kyoto (Île-de-France et outre-mer appartenant à l'UE).

Sources : Citepa ; AIE ; FAO ; Douanes ; Eurostat ; Insee. Traitement : SDES, 2021



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## Several scenarios on the table

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