

LABORATORY NOTEBOOK, COMPUTATIONAL DOCUMENT, REPRODUCIBLE ARTICLE EMACS/ORG-MODE: ONE RING TO RULE THEM ALL?

Arnaud Legrand



MaiMosine, GRICAD, SARI network, June 2023



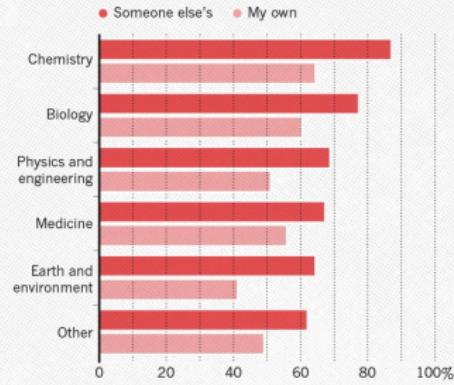
NO TRANSPARENCY NO CONSENSUS



REPRODUCIBILITY "CRISIS": SOCIO-TECHNICAL CHALLENGES

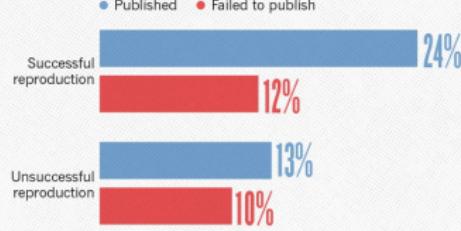
HAVE YOU FAILED TO REPRODUCE AN EXPERIMENT?

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: 1M+ articles per year!
- Emerging practices: DORA/Plan S/COARA, DMP and FAIR data, artefact evaluation, reproducibility badges, reproducibility challenges, open reviews, ...

Methodological/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

DIFFERENT REPRODUCIBILITY CONCERNS IN MODERN SCIENCE

Biology, Oncology sample provenance, clinical trials \rightsquigarrow standardized protocols

Psychology, Nutrition HARKING, p-hacking \rightsquigarrow pre-registration

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Computational fluid dynamics numerical chaos, parallel architectures

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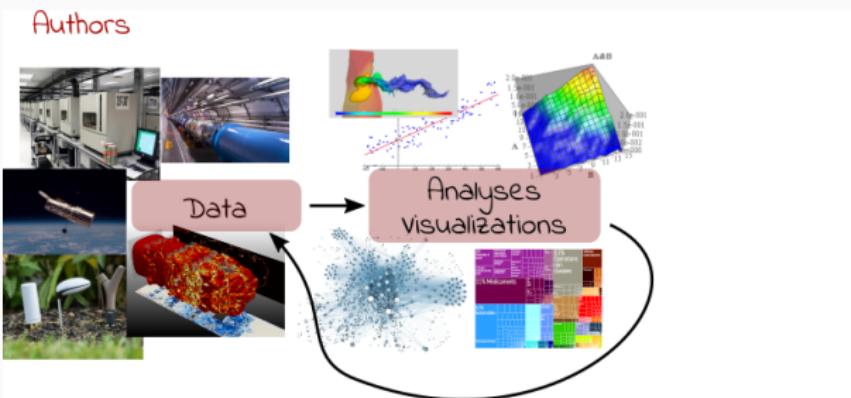
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Artificial Intelligence most of the above 😊

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



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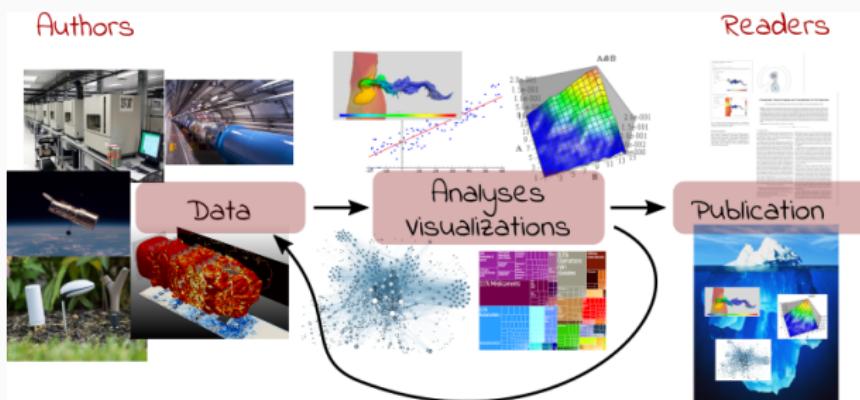
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Reproducible Research = Bridging the Gap by working Transparently

NOTES AND DOCUMENTING

What your research supposedly looks like:

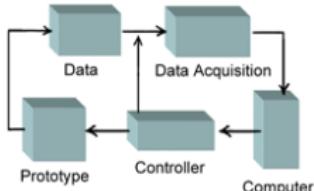


Figure 1. Experimental Diagram

What your research *actually* looks like:

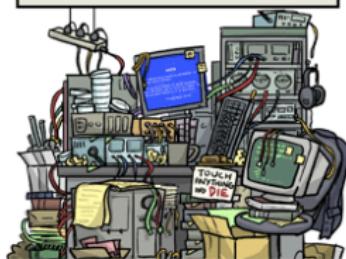


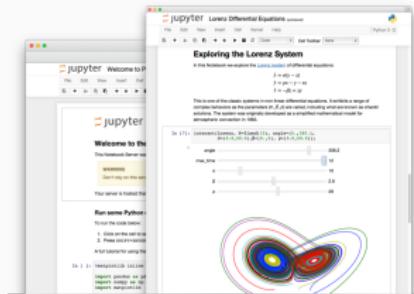
Figure 2. Experimental Mess

JORGE CHAM © 2008

WWW.PHDCOMICS.COM

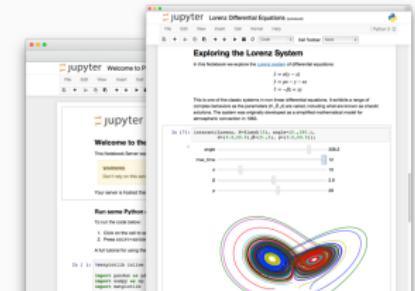
REPRODUCIBILITY ISSUES RELATED TO THE USE OF COMPUTERS

Computation provenance: notebooks and workflows

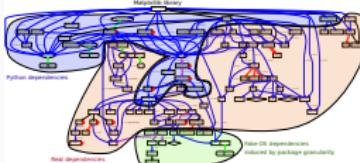


REPRODUCIBILITY ISSUES RELATED TO THE USE OF COMPUTERS

Computation provenance: notebooks and workflows



Software environments

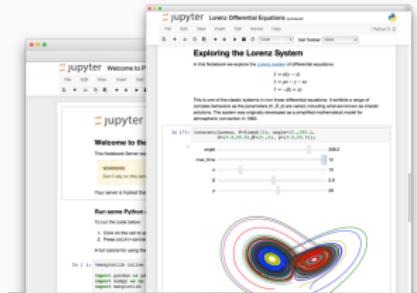


ReproZip



REPRODUCIBILITY ISSUES RELATED TO THE USE OF COMPUTERS

Computation provenance: notebooks and workflows



Software environments



Sharing and Archiving



FRUSTRATION AS AN AUTHOR/REVIEWER



Author (*Calls for a Journal*)

- 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?



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- **It worked yesterday!** 6 months later: **Why did I do that?**

Reviewer (Calls for a *Reproducible Article*)

- 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/LITERATE PROGRAMMING

Un document computationnel

Mon ordinateur m'indique que π vaut approximativement

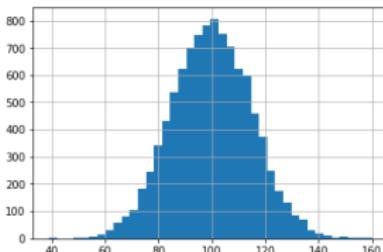
3.141592653589793

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

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

3.1437198694098765

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



TOOL 1: COMPUTATIONAL NOTEBOOKS/LITERATE PROGRAMMING

Document initial dans son environnement

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

- In [1]:** `# Un document computationnel`
Output: Mais ordinateur m'indique que π vaut "approximativement"
- In [1]:** `from math import *`
Output: 3.141592653589793
- In [2]:** `Mais calculé avec la méthode des aiguilles de Buffon (https://fr.wikipedia.org/wiki/Aiguille_de_Buffon), on obtient d'autant 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`
Output: 3.14371986944998765
- In [3]:** `On peut inclure des formules mathématiques comme $\sqrt{2/\pi} \exp(-x^2/2)$ et des dessins qui n'ont rien à voir avec π (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()`
Output: A histogram showing a bell-shaped distribution centered at 100, with a peak frequency of approximately 800.

Document final

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3.141592653589793

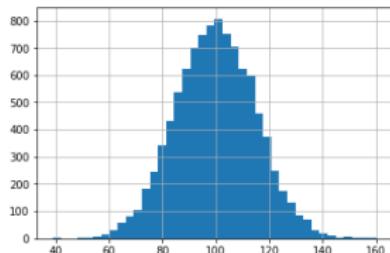
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2/(sum((x+np.sin(theta))>1)/N)
```

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

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TOOL 1: COMPUTATIONAL NOTEBOOKS/LITERATE PROGRAMMING

Document initial dans son environnement

Jupyter example_pl (modified)

Un document computationnel

Mais mon ordinateur m'indique que π 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), 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 π (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

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Mon ordinateur m'indique que π vaut approximativement

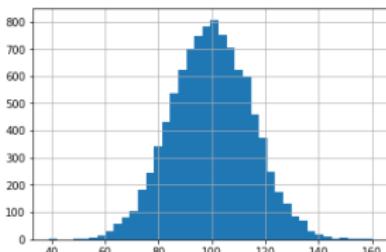
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Mais calculé avec la [méthode des aiguilles de Buffon](#), on obtient comme approximation :

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TOOL 1: COMPUTATIONAL NOTEBOOKS/LITERATE 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 has three cells:

- In [1]:** `# Un document computationnel`. The output shows the value of pi as 3,141592653589793.
- In [2]:** A code cell with imports for numpy and random, calculating pi using Buffon's needle method. The output shows the result 3.1437198694098765.
- In [3]:** A code cell with imports for numpy, matplotlib, and random, creating a histogram of 100,000 random numbers. The output is a histogram plot centered around 100.

Document final

Un document computationnel

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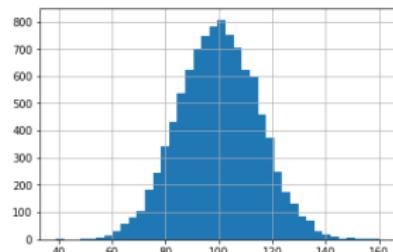
Mais calculé avec la **méthode des aiguilles de Buffon**, on obtiendrait comme approximation :

```
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N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
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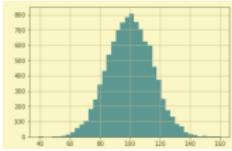
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In [1]:  
from math import *  
print(pi)  
3.141592653589793
```

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

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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  
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 π (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

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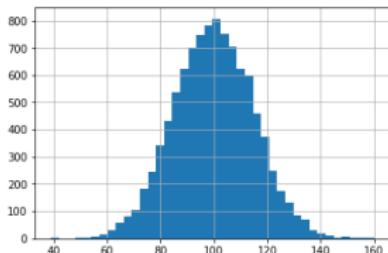
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TOOL 1: COMPUTATIONAL NOTEBOOKS/LITERATE PROGRAMMING

Document initial dans son environnement

Un document computationnel

```
In [1]: from math import * print(pi) 3,141592653589793
```

Mais calculé avec la `_methodes_ des éimpulles de Buffon` (https://fr.wikipedia.org/wiki/Algille_de_Buffon), on obtiendrait comme `approximation` :

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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 3,1437198694098765
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```
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

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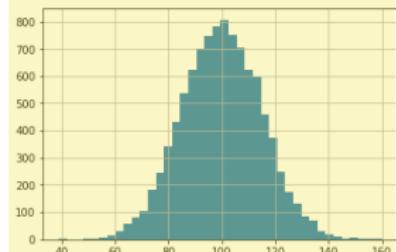
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```

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 π (si ce n'est une constante de normalisation... ☺).



TOOL 1: COMPUTATIONAL NOTEBOOKS/LITERATE 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, y) and calculates the ratio of points below the unit circle to the total number of points to approximate pi.
- In [3]:** Plots a histogram of a normal distribution with mean 100 and standard deviation 15, showing a bell-shaped curve.

Document final

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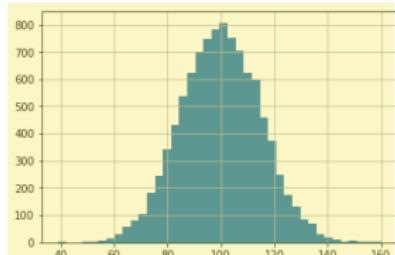
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SEVERAL POSSIBLE USAGES

Code Documentation (\neq code comments)

- For developers: explain code organization (data structures, algorithms, modules, class, etc.) and how to contribute
- For users: API, examples, installation, ...

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Data Analysis data dependent

- Data transformation/curation
- Exploratory/sequential data analysis
- Document hypothesis, graphs/tables

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Reproducible article (book with code/computations)

- Classical article/book structure with typography constraints
- Code is behind the scene (e.g., figures, tables, numbers)

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"Laboratory" notebook Research reporting. Daily notes on

- Experimental parameters, specific configurations
- Meetings, seminars, lectures, ...
- Readings, bibliography
- TODOs, Ideas, Random hacks

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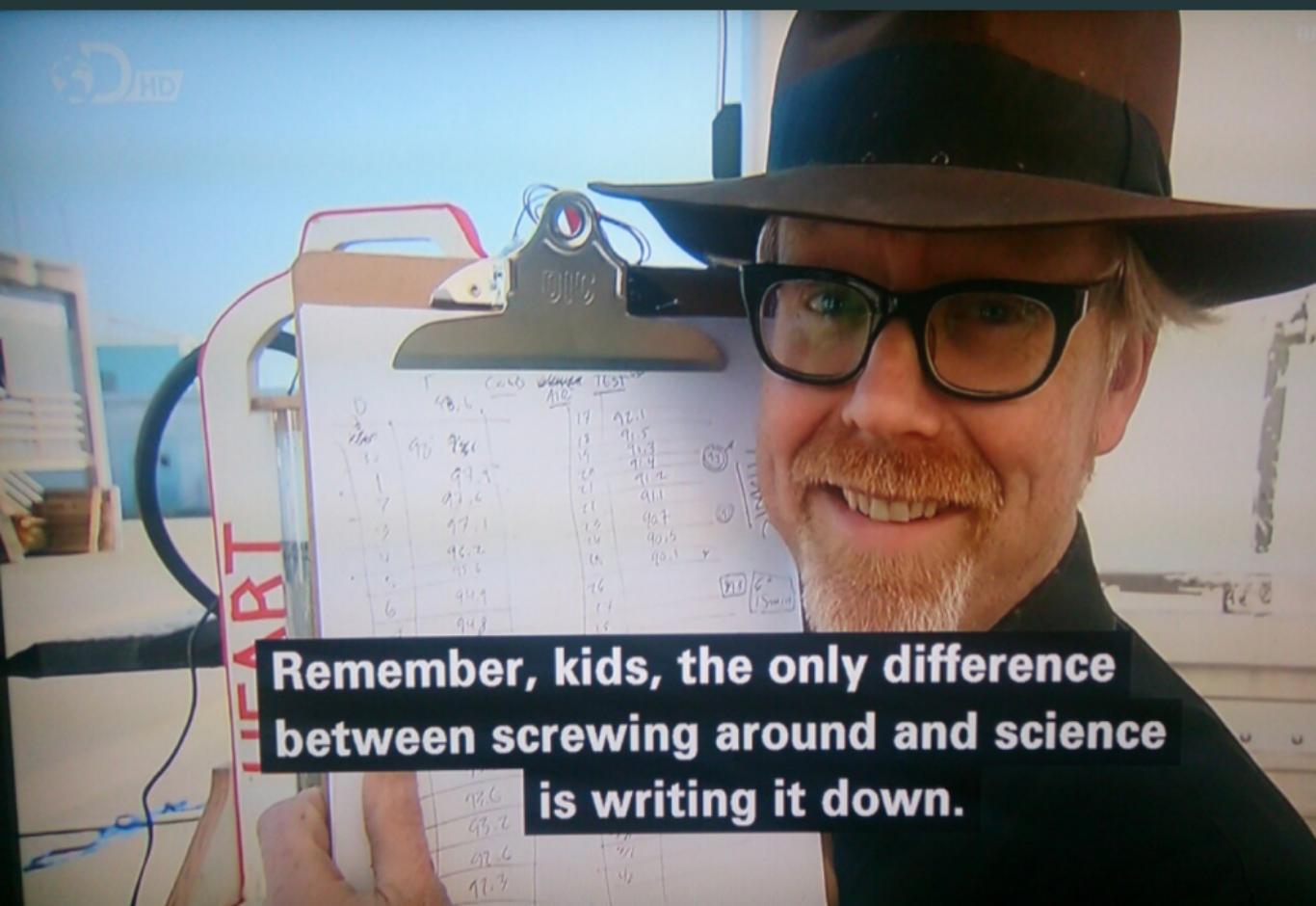
"Laboratory" notebook Research reporting. Daily notes on

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Teaching material, Presentations

Dynamic documents, Websites, ...

LABORATORY NOTEBOOKS, COMPUTATIONAL DOCUMENTS



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

QUICK DEMO OF JUPYTER, RSTUDIO, AND ORG-MODE



(python)

Pros Python/R, friendly, portable (web browser, client/server)

- Cons**
- Installation, software dependencies (`minimal-notebook` \approx 440Mb)
 - Limited control on typography (unless using *Rube Goldberg* machines like <https://quarto.org/>)

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Studio[®] (java/R)

Pros R/Python, friendly, portable, real IDE, Good typography control

- Cons**
- Installation, software dependencies (`rocker/rstudio` \approx 550Mb)
 - Limited control on typography (unless using monsters like `quarto`)

QUICK DEMO OF JUPYTER, RSTUDIO, AND ORG-MODE



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(emacs-lisp)

Pros R, Python, Perl, Ruby, C, Java, ...

- Pure text, Good typography control, "Lightweight", Programmable editor

Cons

- No default configuration \leadsto rough and steep learning curve
- Big machinery: `silex/emacs-alpine-ci` \approx 240Mb even though `flycheck/emacs-cask` \approx 80Mb

WHICH TOOL FOR WHICH USAGE ?

A biased opinion

	Jupyter
Coding	
Data Analysis	
Articles	
Lab Notebook	
Slides	
Dynamic docs	
Websites	

WHICH TOOL FOR WHICH USAGE ?

A biased opinion

	Jupyter	Rstudio
Coding	:(:((R)
Data Analysis	:)	:)
Articles	:(:)
Lab Notebook	:(:)
Slides	:	:)
Dynamic docs	:)	:)
Websites		

WHICH TOOL FOR WHICH USAGE ?

A biased opinion

	Jupyter	Rstudio	Org-mode
Coding	😢	😊 (R)	😐
Data Analysis	😎	😎	😊
Articles	😢	😊	😈
Lab Notebook	😢	😐	😈
Slides	😐	😊	😊
Dynamic docs	😎	😊	😢
Websites			

PANDORA'S BOX



COMMON ISSUES

1. Format evolution through time (increasing complexity)

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2. Environment control. Uuh ???



COMMON ISSUES

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3. Scalability

REPRODUCIBLE RESEARCH = RIGOR AND TRANSPARENCY

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

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

- Konrad Hinsen, Christophe Pouzat
- 3rd Edition: March 2020 – March 2023 (15,000+)



REPRODUCIBLE RESEARCH = RIGOR AND TRANSPARENCY

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MOOC "Advanced RR" planned for Nov. 2023

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- Software environment control (`docker, singularity, guix`)
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4. Prepare the Future:

- Reuse, reuse, reuse!
- Toward **literate experimentation?**
- Shared and controlled testbeds
- How to **share** Experiments/Simulations ?



THE SCIENCE IS CLEAR

Why are we
ignoring it?

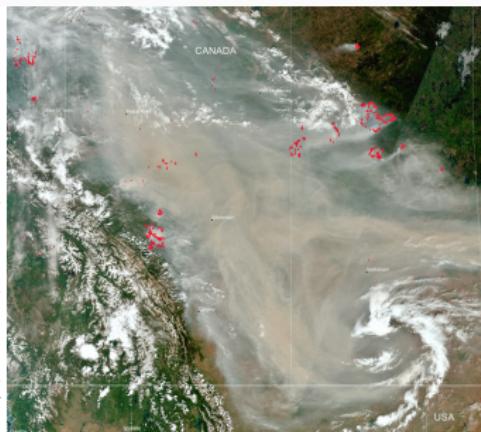
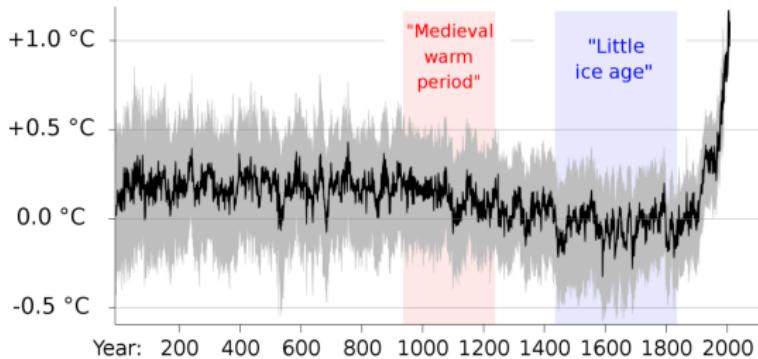
scientist rebellion

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

1. Global climate change is not a future problem



Global Average Temperature Change



https://en.wikipedia.org/wiki/Global_temperature_record

2023 Alberta wildfires (> 1 Mha)

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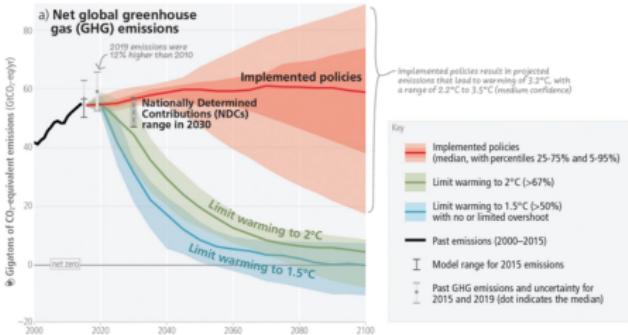


IPCC, IPBES, <https://climate.nasa.gov/>

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

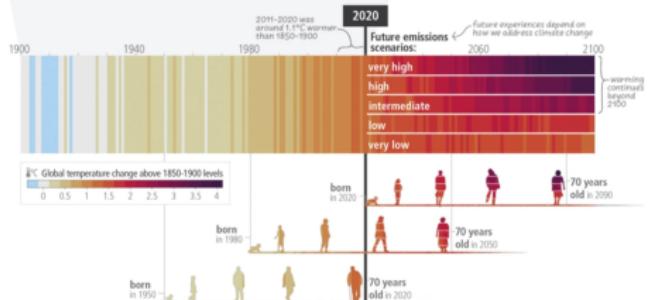
Limiting warming to 1.5°C and 2°C involves rapid, deep and in most cases immediate greenhouse gas emission reductions

Net zero: CO₂ 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



Latest IPCC report

14/15

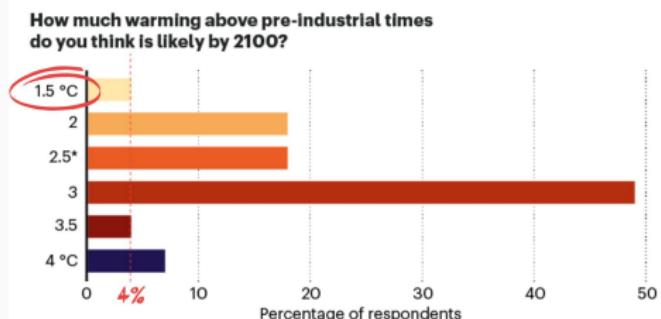
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3. **9 out of 10 IPCC scientists believe overshoot is likely**

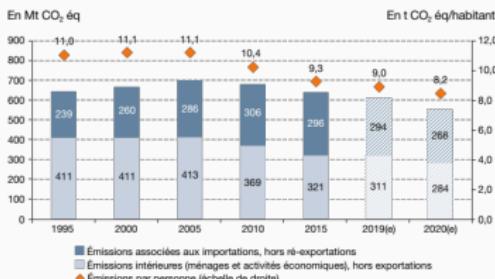


@natu Nature survey, Nov. 2021

THE ELEPHANT IN THE ROOM: CLIMATE CHANGE

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

ÉVOLUTION DE L'EMPREINTE CARBONE DE LA FRANCE



(e) = estimations.

Note : l'empreinte carbone porte sur les trois principaux gaz à effet de serre (CO₂, CH₄, N₂O). 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'ensemble de la série a ainsi été révisé, l'essentiel des ajustements portant sur les émissions importées de CH₄.

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

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

Empreinte carbone moyenne en France 10 tonnes de CO₂e/an/pers.



$\div 2$
d'ici
2030

<2t CO₂e

Objectif d'ici 2050

- de 2 t de CO₂e/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 CO₂e/Annee : à la maison, préférence à ses produits régionaux

0,5 t CO₂e/Annee : faire une partie route (300km) de votre voiture ancienne sur 30 ans, risquez de faire un peu moins de km dans les transports en commun.

0,5 t CO₂e/Annee : faire du vélo, prendre le bus ou le métro, faire des emplacements décentralisés et intermodaux, se servir dans des magasins locaux et locaux

0,2 t CO₂e/Annee : échapper au chauffage sur un an (IPCC en parle, "0°C" c'est l'effort d'un changement basé sur le climat pour éviter la catastrophe mondiale)

0,2 t CO₂e/Annee : faire un peu moins de km en voiture, mais pas à chaque fois, par exemple à la course ou sociale mentale

0,2 t CO₂e/Annee : faire des emplacements décentralisés et intermodaux, se servir dans des magasins locaux et locaux

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

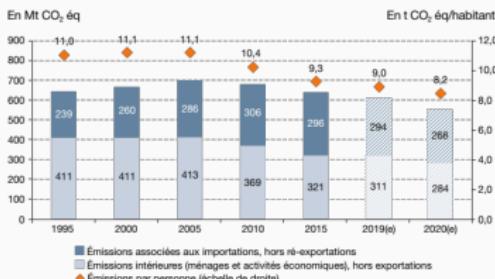
INVENTONS
NOS VIES
BAS CARBONE

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

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

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Par exemple :

1. Changer d'alimentation : à tendance végétalienne, hyperproteïne et sans produits animaux

2. Changer de transport : 2000km en voiture (800kg), de fabrication anonyme sur 30 ans, importation de denrées et déchets, dépendance au pétrole, transports en commun

3. Changer d'habitation : ériger rien de tout, mais faire des aménagements décentralisés et intergénérationnels, sobriété dans l'usage des ressources

4. Changer d'agriculture : Choisir bio sur un critère

en priorité, "l'offre" n'est pas d'un agriculteur bien isolé mais d'un système qui fonctionne à plusieurs échelles et socialement équilibré

5. Changer de services publics : faire évoluer, simplifier, optimiser, faire évoluer vers une société moins consommatrice et plus solidaire

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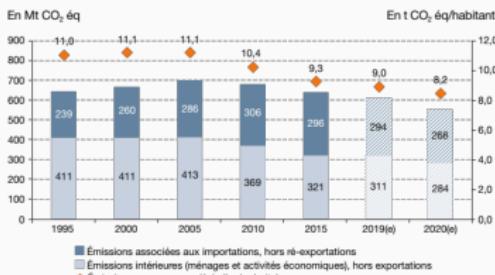
French government response

- 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

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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