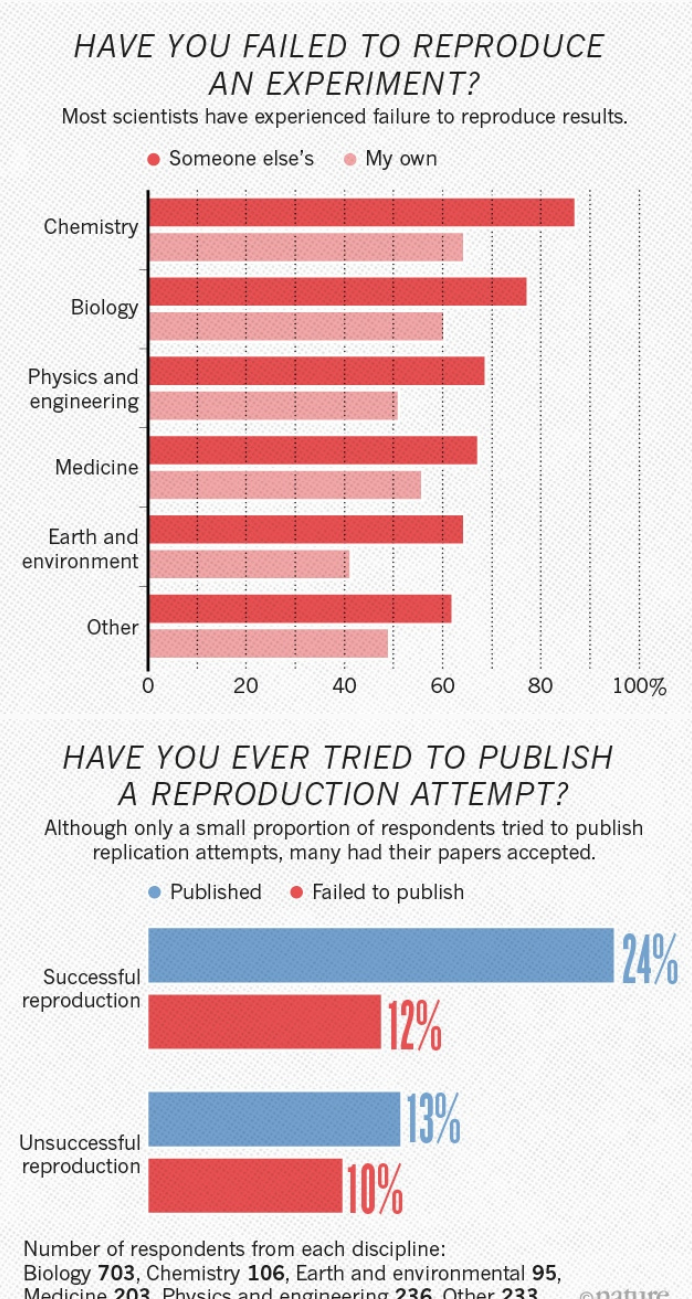
Laboratory notebook, computational document, reproducible article
Emacs/Org-mode: One ring to rule them all?

Arnaud Legrand

MaiMosine, GRICAD, SARI network, June 2023

Reproducibility "Crisis": Socio-technical Challenges



1,500 scientists lift the lid on reproducibility, Nature, May 2016

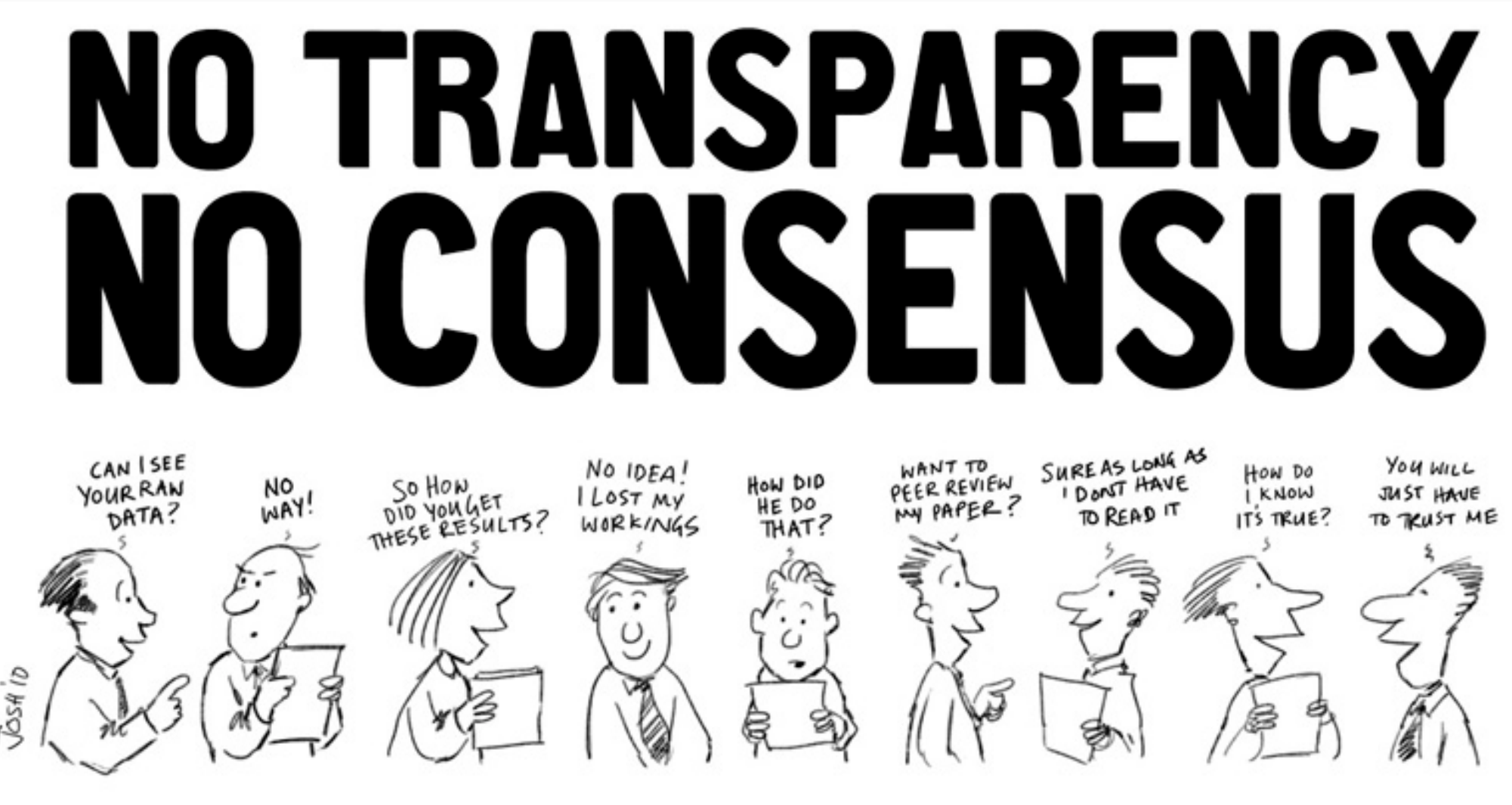
Social causes

- 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

Scientific Consensus



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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Artificial Intelligence most of the above 😉

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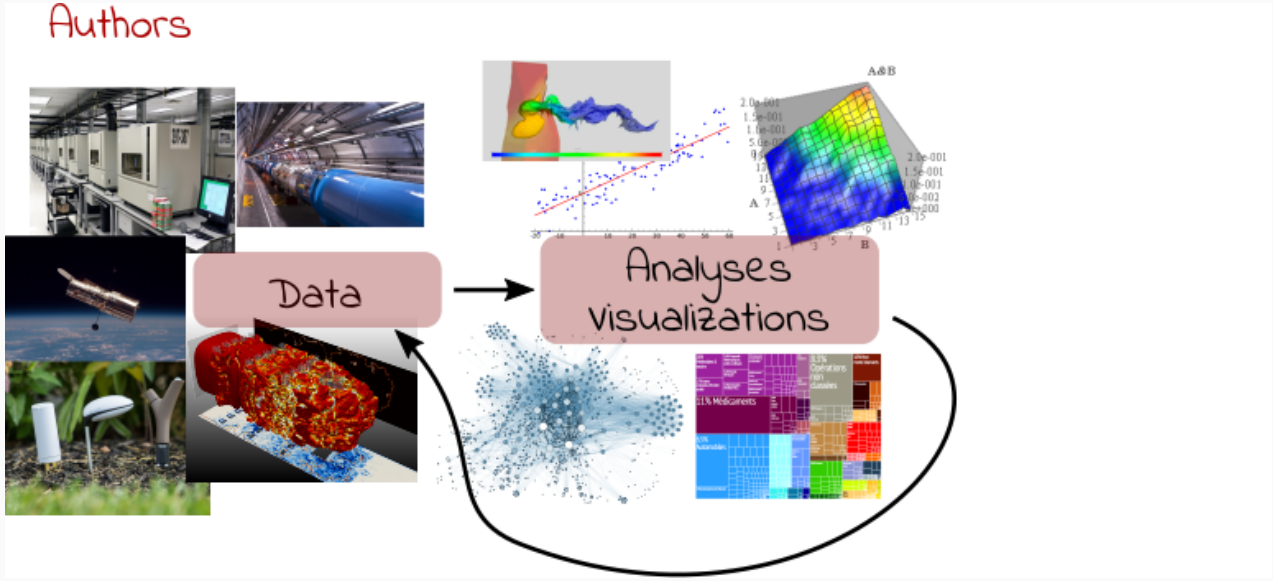

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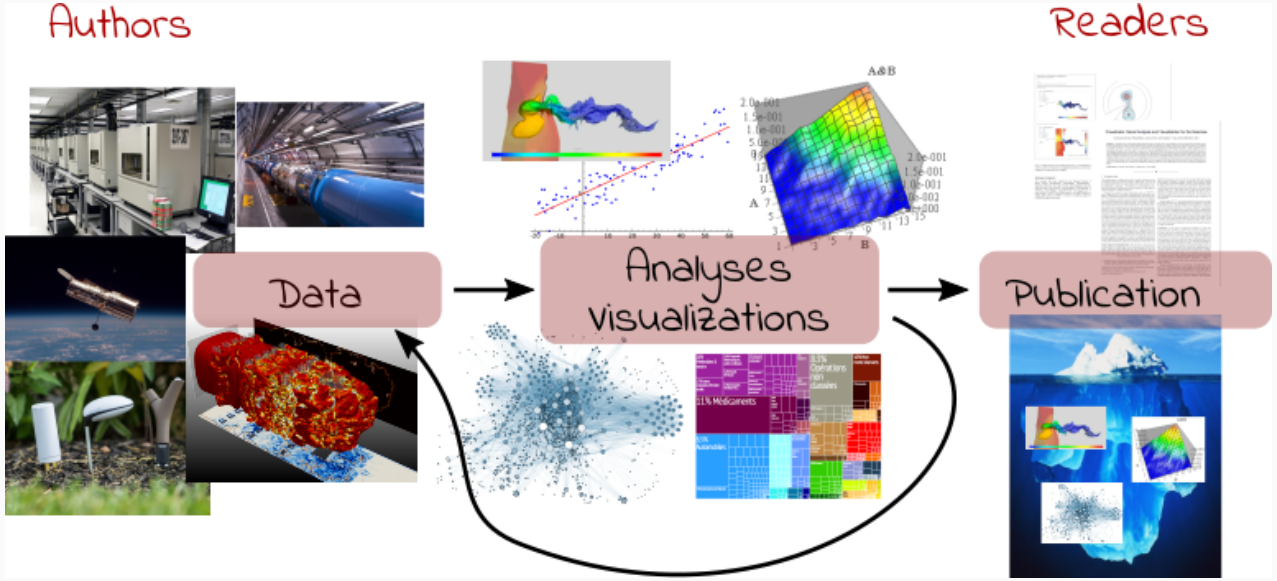
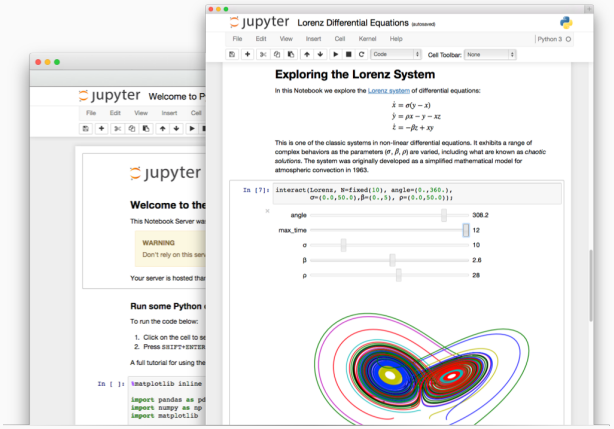


Reproducible Research = Bridging the Gap by working Transparently

Reproducibility Issues Related to the use of Computers

Computation provenance: notebooks and workflows



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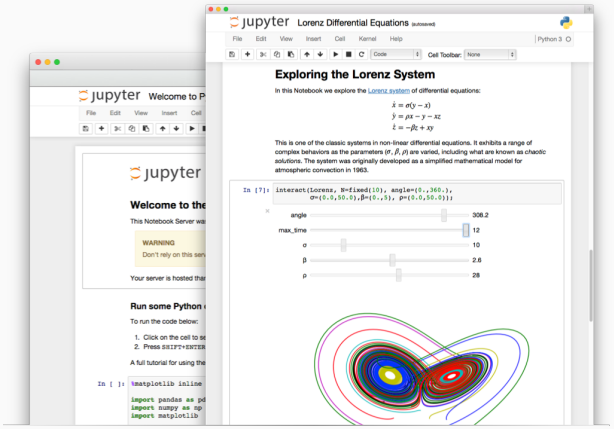

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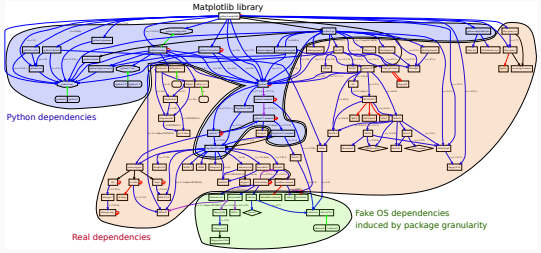

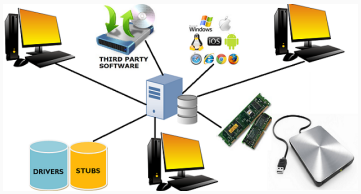

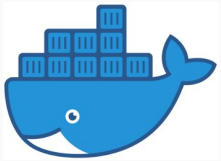

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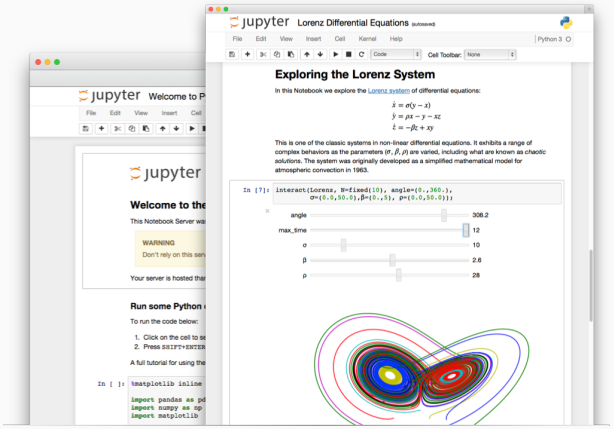

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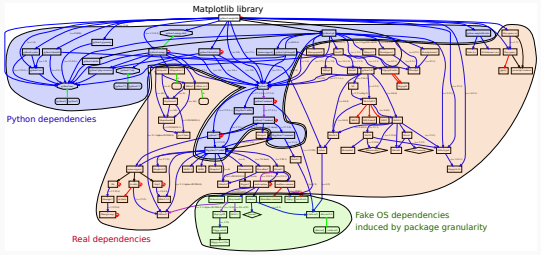

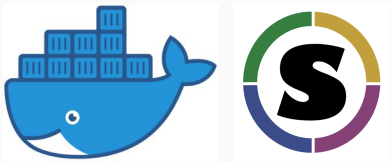

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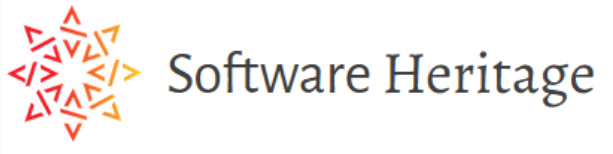


Good Practice #1

Taking Notes and Documenting

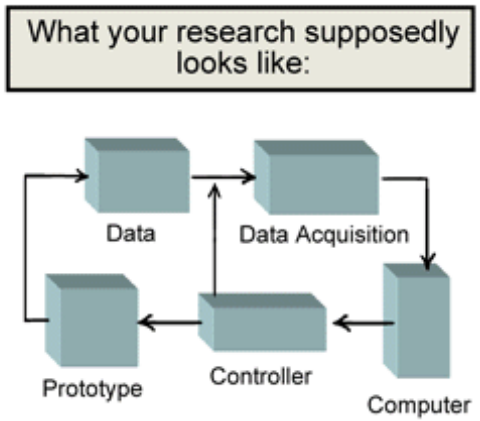


Figure 1. Experimental Diagram

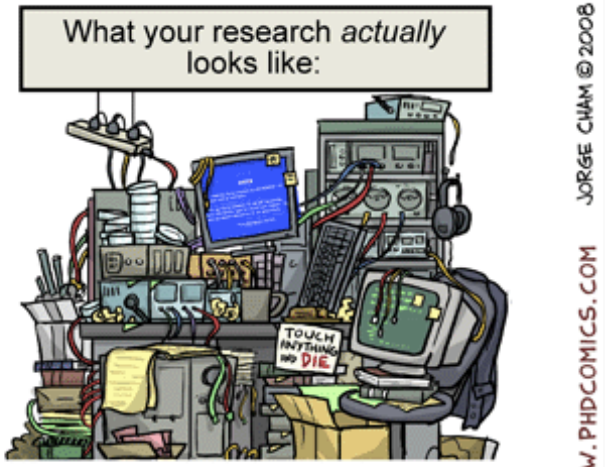
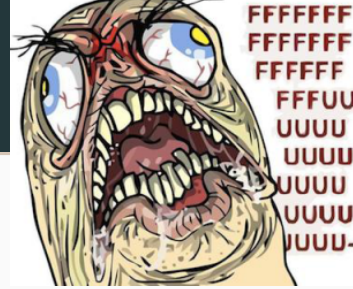


Figure 2. Experimental Mess

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?
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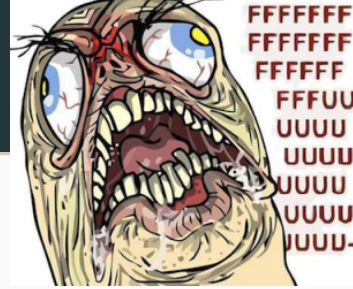

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Reviewer (Calls for a *Reproducible Article*)

- 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*

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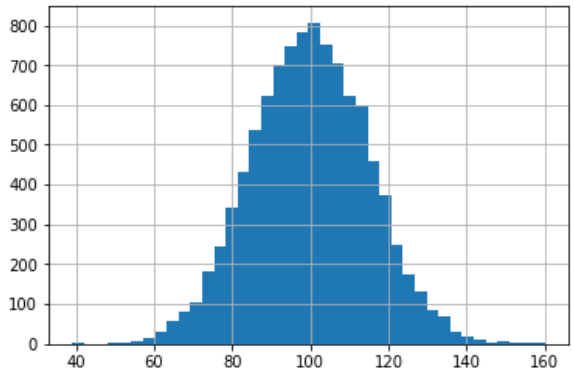

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jupyter example_pi (autosaved)

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Code CellToolbar

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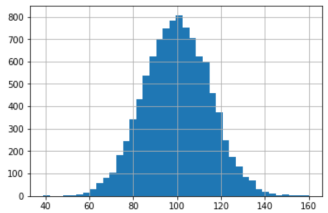

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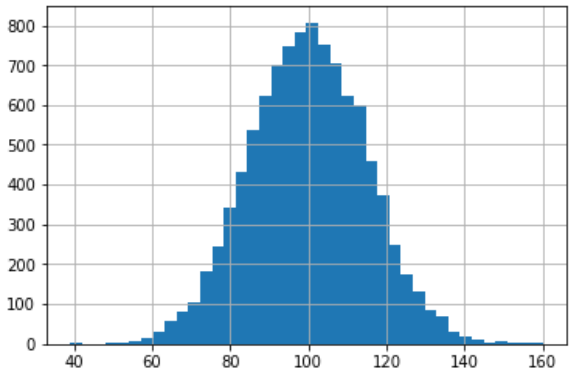

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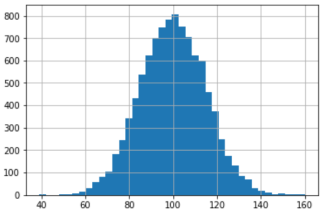

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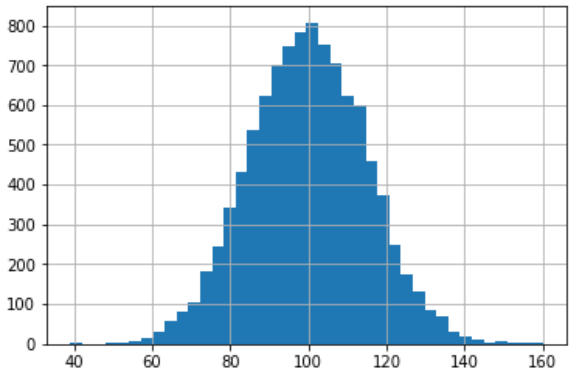

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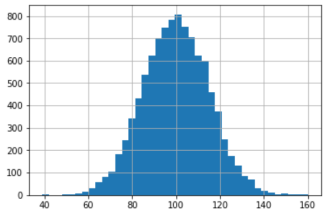

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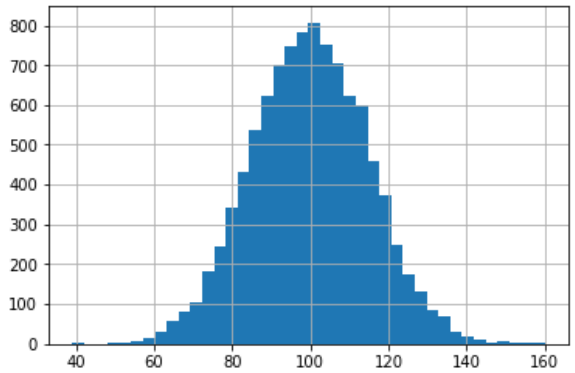

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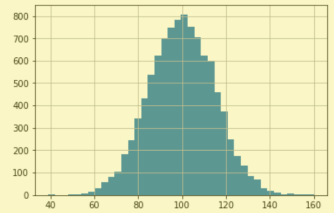

Résultats

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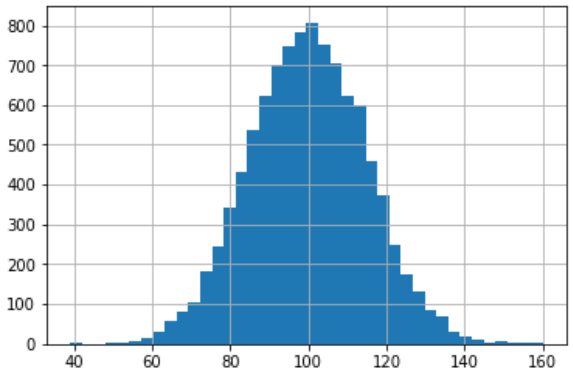

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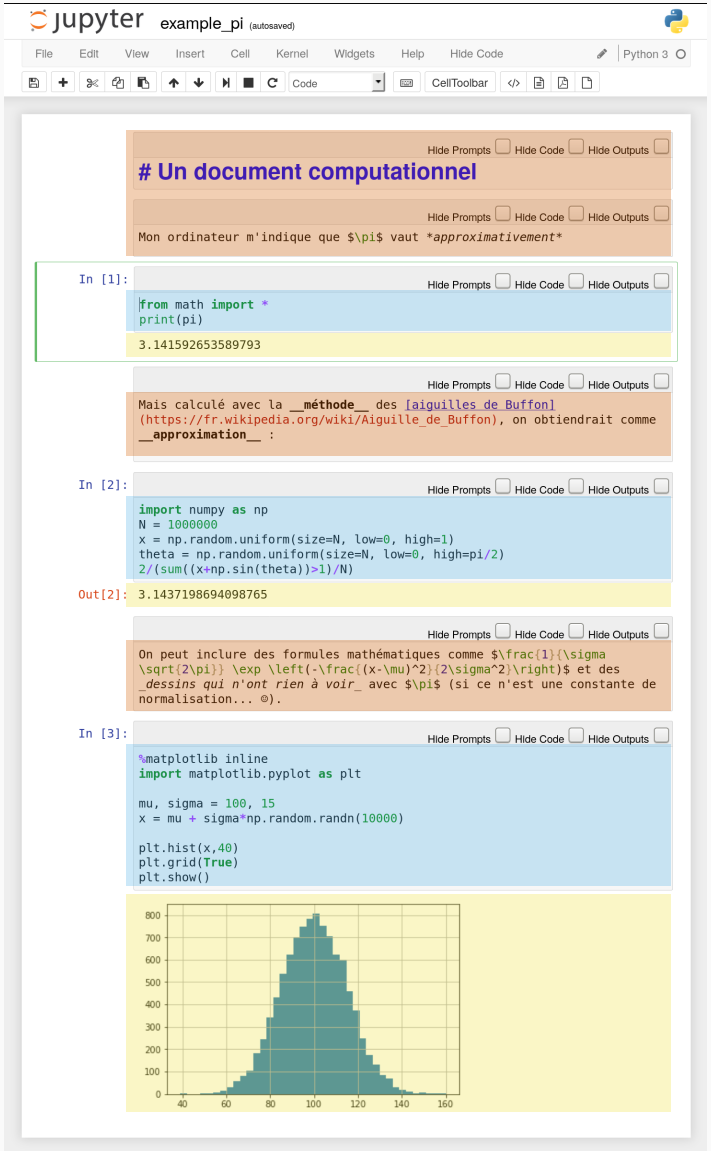

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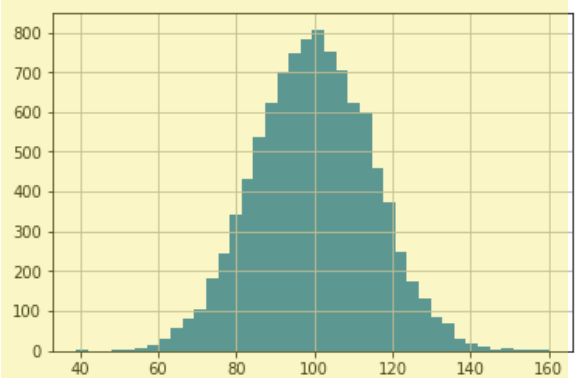
N = 1000000
x = np.random.uniform(size=N, low=0, high=1)
theta = np.random.uniform(size=N, low=0, high=pi/2)
2/(sum((x+np.sin(theta))>1)/N)
```

```
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

jupyter example_pi (autosaved)

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

Code CellToolbar

Hide Prompts Hide Code Hide Outputs

```
# Un document computationnel
```

Hide Prompts Hide Code Hide Outputs

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

In [1]:

Hide Prompts Hide Code Hide Outputs

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

```
3.141592653589793
```

Hide Prompts Hide Code Hide Outputs

```
Mais calculé avec la __méthode__ des [aiguilles de Buffon]
(https://fr.wikipedia.org/wiki/Aiguille_de_Buffon), on obtiendrait comme
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Hide Prompts Hide Code Hide Outputs

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Out[2]: 3.1437198694098765

Hide Prompts Hide Code Hide Outputs

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```

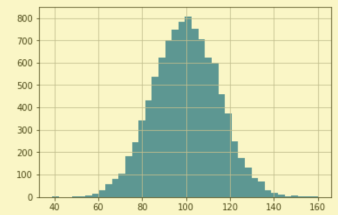
In [3]:

Hide Prompts Hide Code Hide Outputs

```
%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()
```



Export

Document final

Un document computationnel

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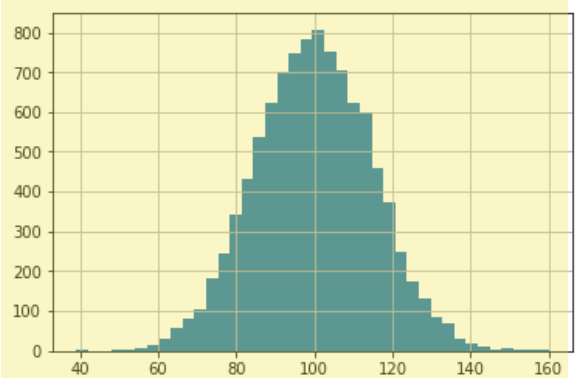

Several possible usages

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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- Exploratory/sequential data analysis
- Document hypothesis, graphs/tables

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"Laboratory" notebook Research reporting. Daily notes on

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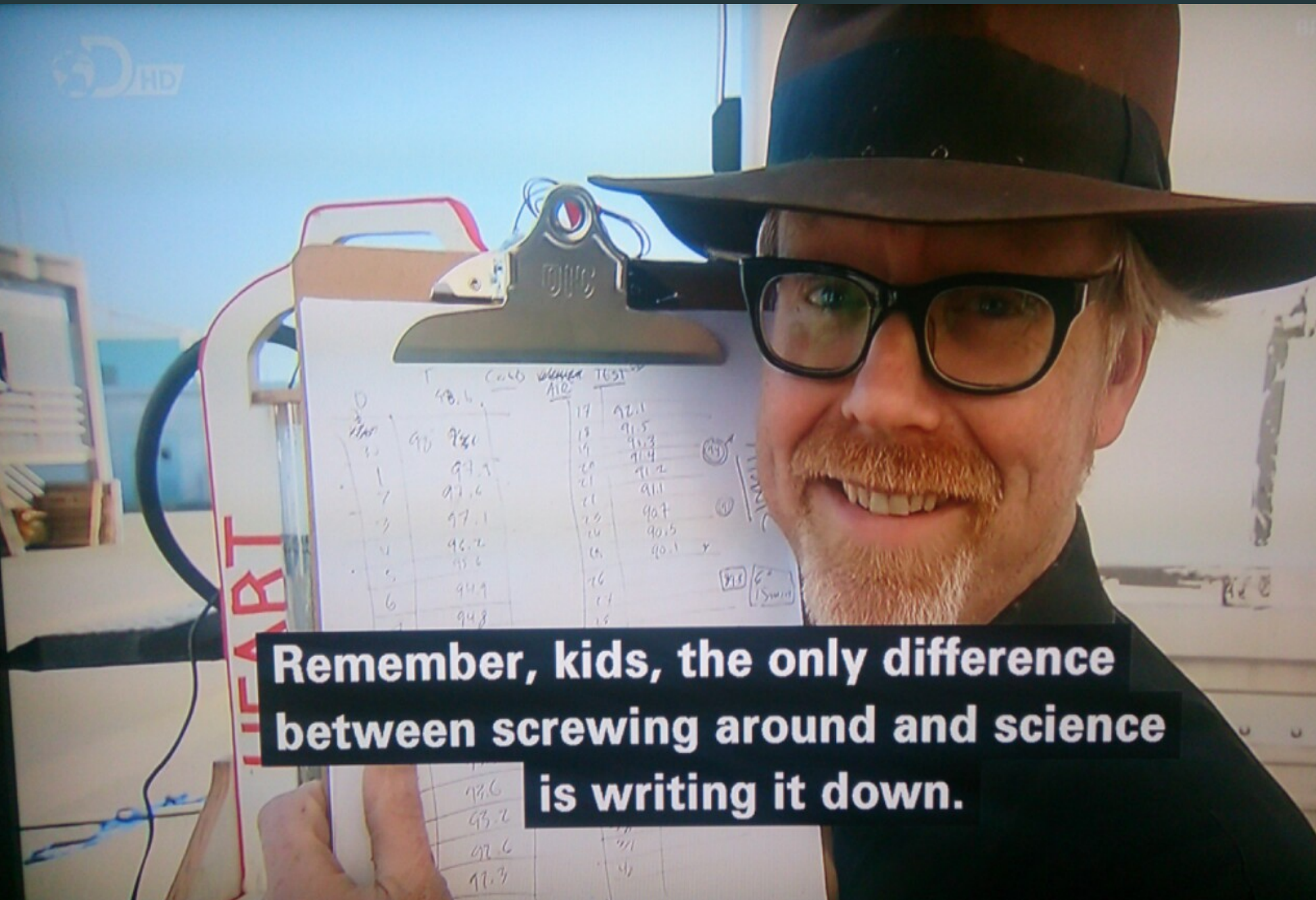
Teaching material, Presentations

Dynamic documents, Websites, ...

Laboratory Notebooks, Computational Documents



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)
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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 ⇝rough and steep learning curve
- Big machinery: silex/emacs-alpine-ci ≈ 240Mb even though flycheck/emacs-cask ≈ 80Mb

Which tool for which usage ?

A biased opinion

	Jupyter
Coding	
Data Analysis	
Articles	
Lab Notebook	
Slides	
Dynamic docs	
~~Websites~~	

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Pandora's box

Common Issues

1. Format evolution through time (increasing complexity)

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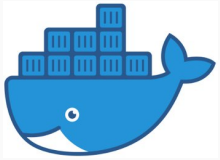

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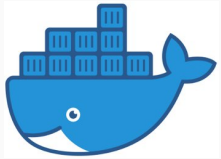

3. Scalability

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

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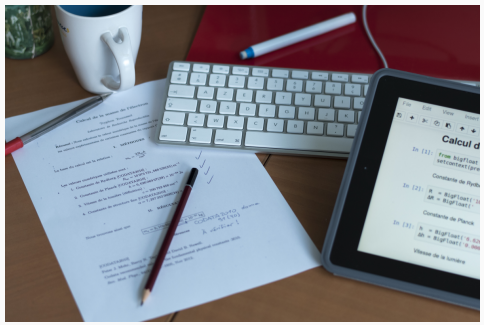

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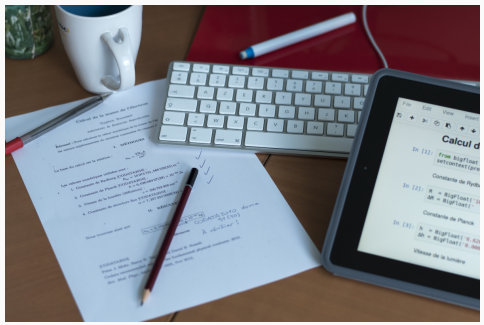

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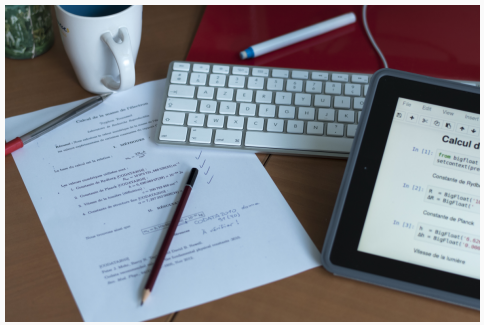

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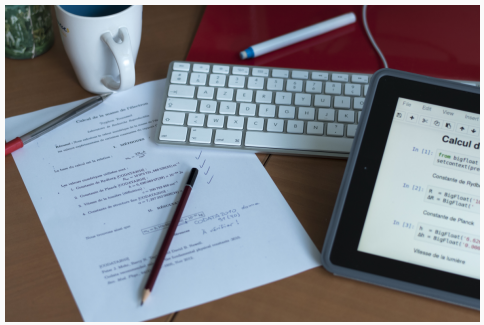

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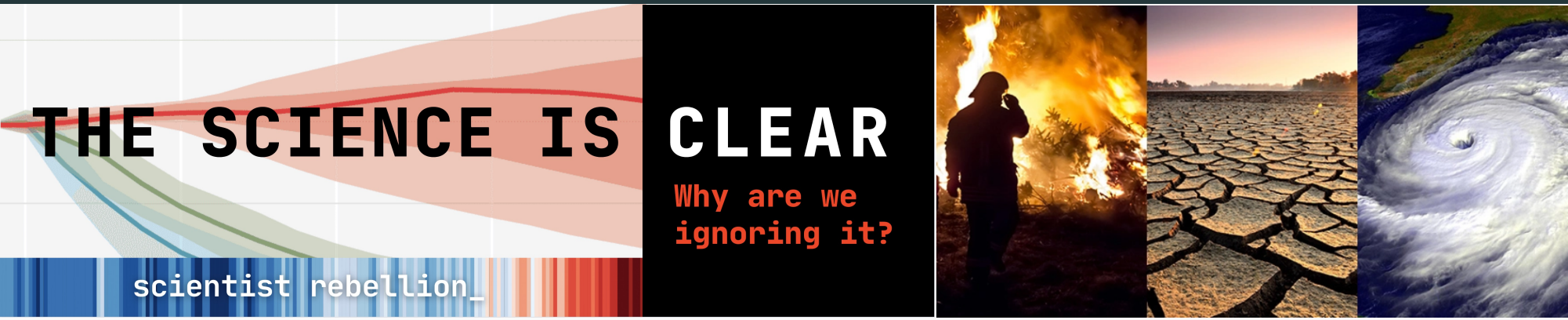
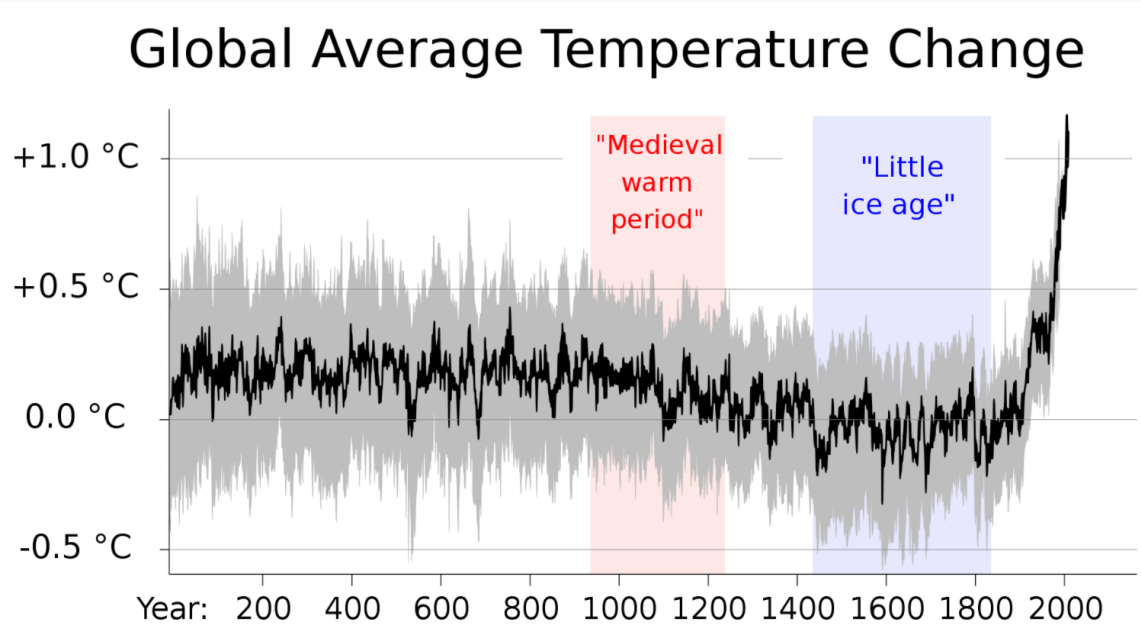
4. **Prepare the Future:**
   - Reuse, reuse, reuse!
   - Toward literate experimentation?
   - Shared and controled testbeds
   - How to share Experiments/Simulations ?

The Elephant in the Room: Climate Change

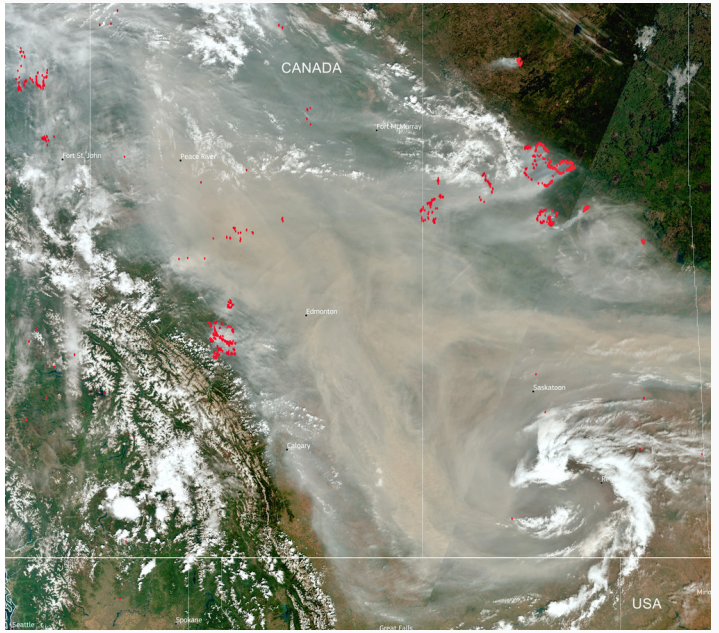


IPCC, IPBES, https://climate.nasa.gov/

1. Global climate change is **not** a future problem

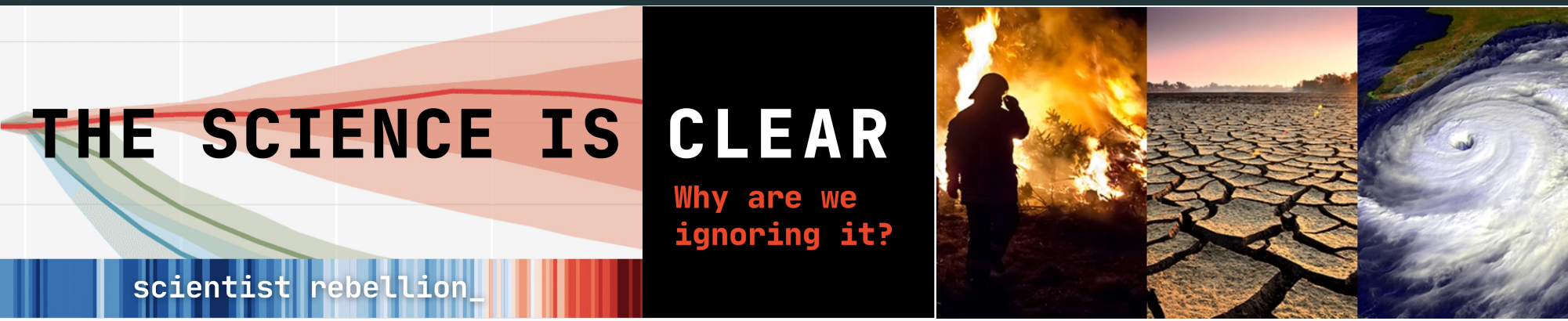


https://en.wikipedia.org/wiki/Global_temperature_record



2023 Alberta wildfires (> 1 Mha)

The Elephant in the Room: Climate Change



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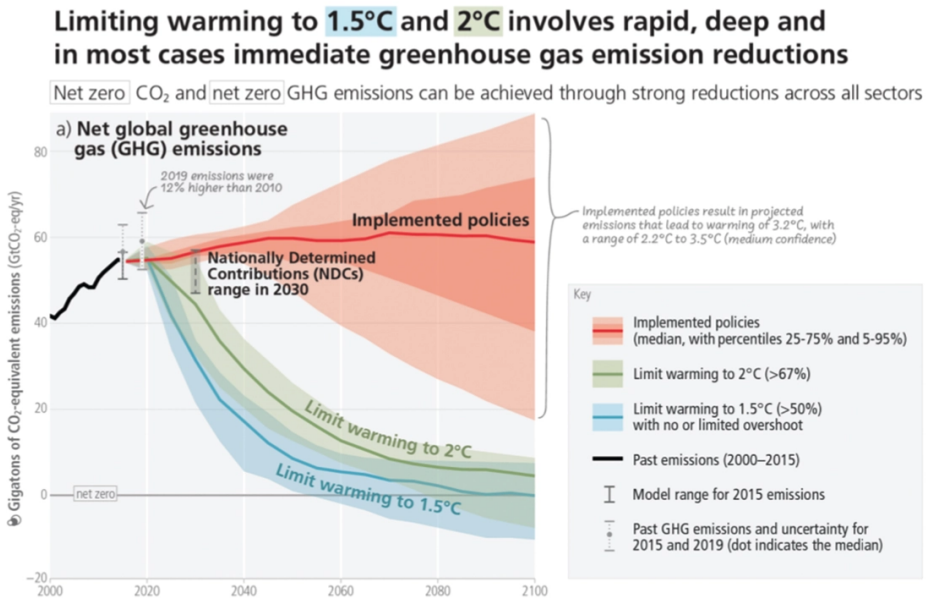
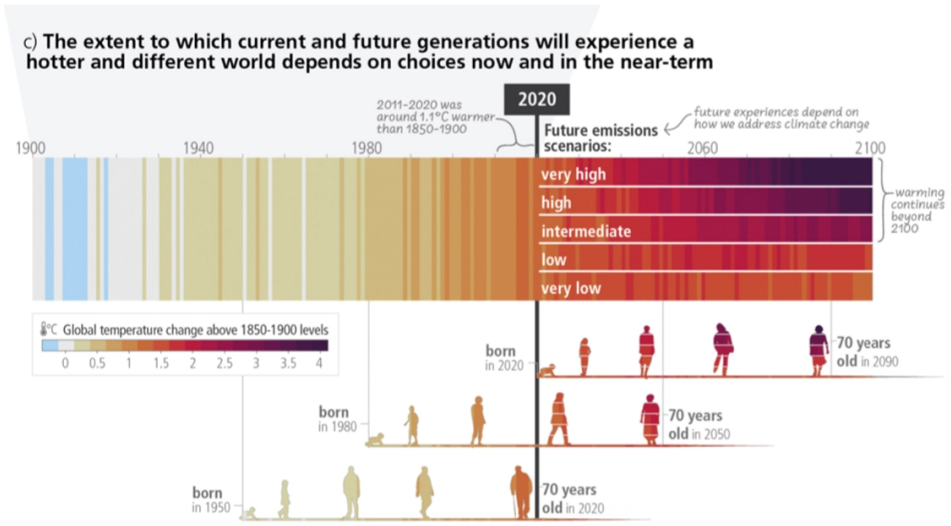
1. Global climate change is **not** a future problem
2. It is **entirely** due to human activity

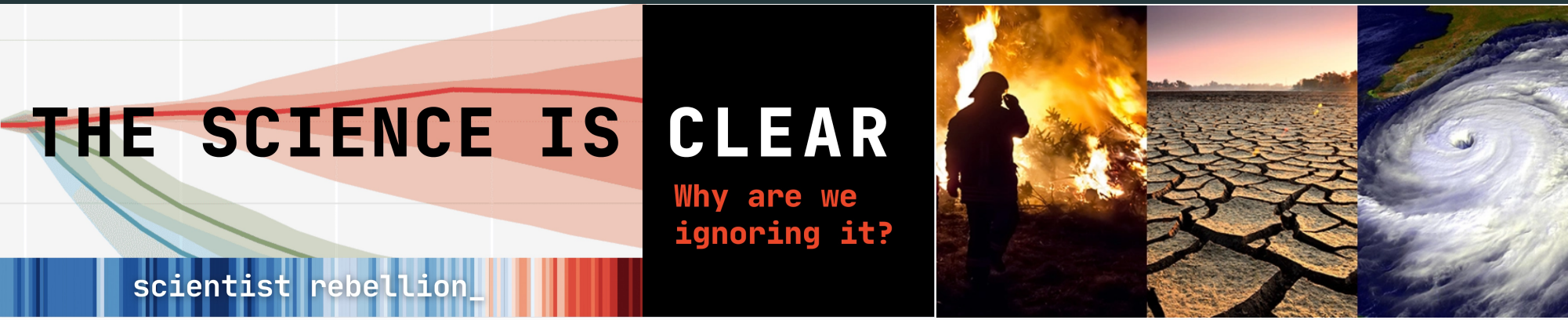




Paris Agreement'15 ∼ Net Zero by 2050

Latest IPCC report

The Elephant in the Room: Climate Change



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

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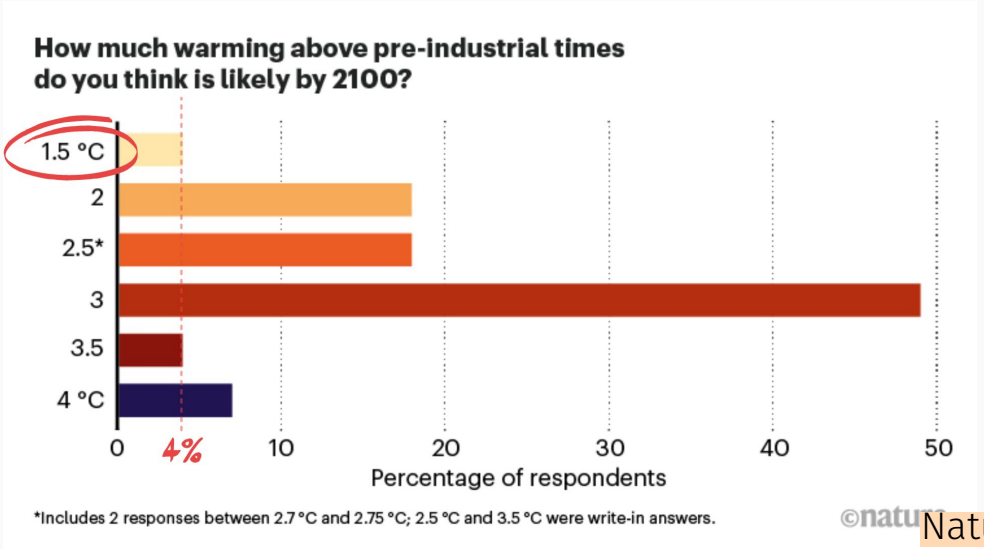
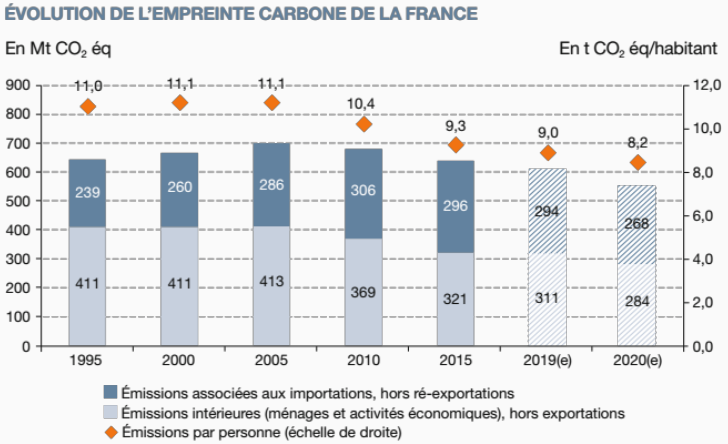
3. *9 out of 10 IPCC scientists believe overshoot is likely*

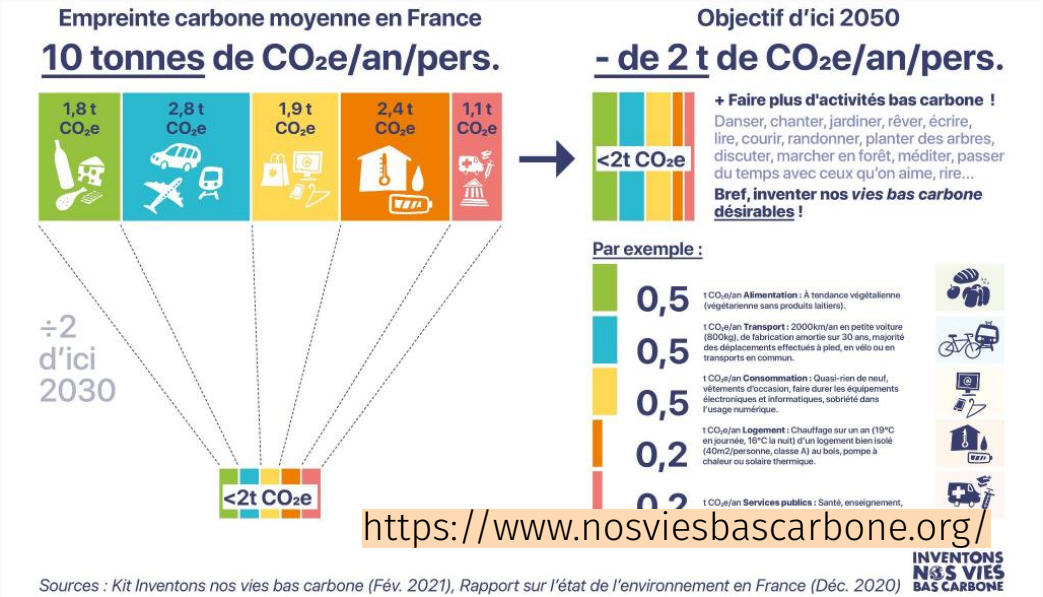


Nature survey, Nov. 2021

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



(e) = estimations.
Note : l'empreinte carbone porte sur les trois principaux gaz à effet de serre (CO_2, CH_4, N_2O). 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 révisée, l'essentiel des ajustements portant sur les émissions importées de CH_4.
Champ : périmètre Kyoto (métropole et outre-mer appartenant à l'UE).
***Sources :** Citepa ; AIE ; FAO ; Douanes ; Eurostat ; Insee. Traitement : SDES, 2021*



https://www.nosviesbascarbone.org/

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

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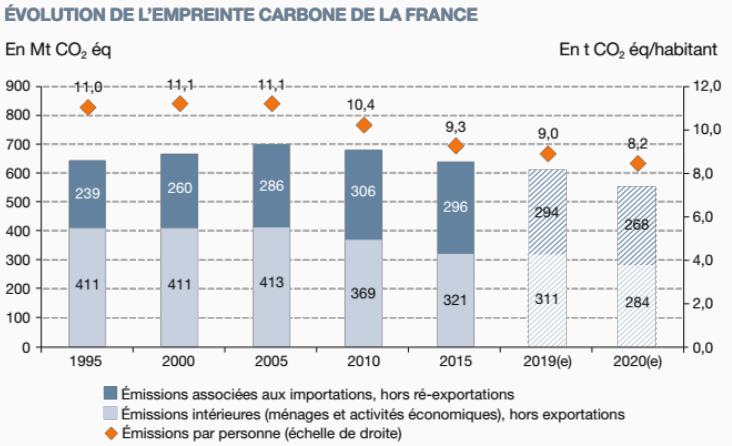

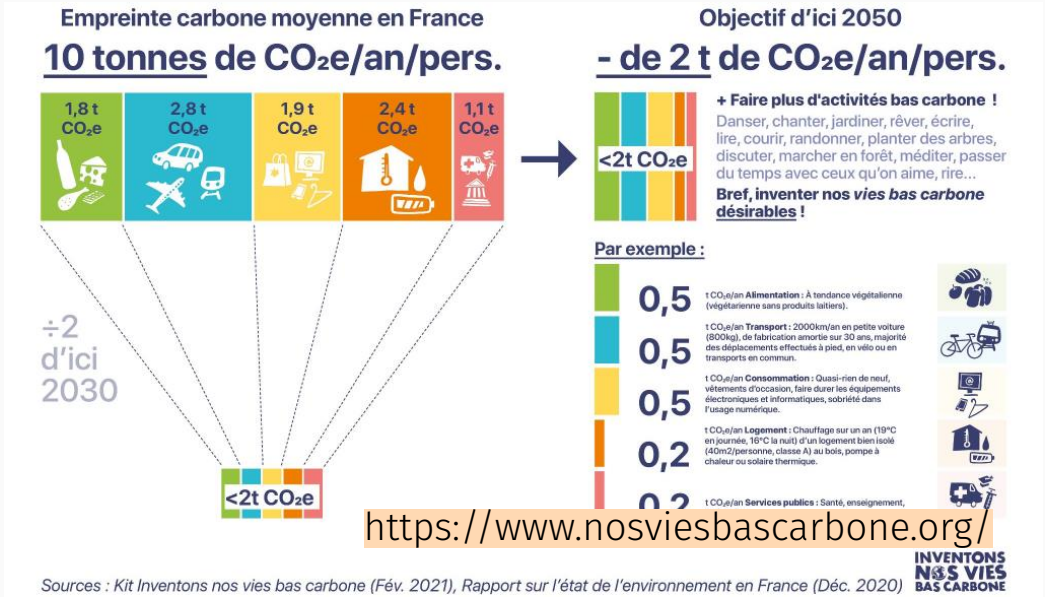

French government response

- *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

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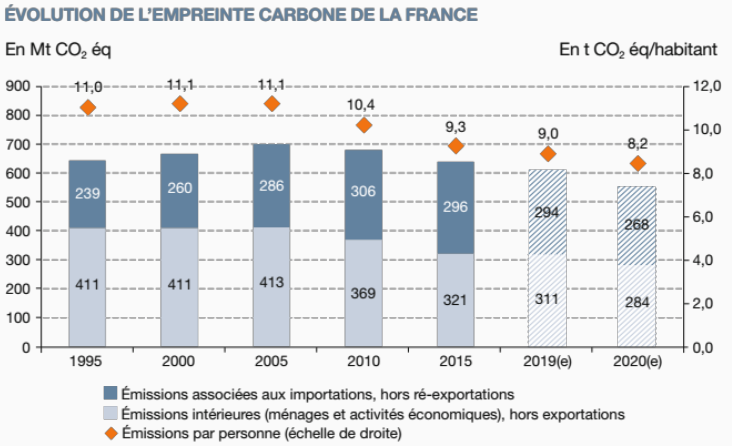

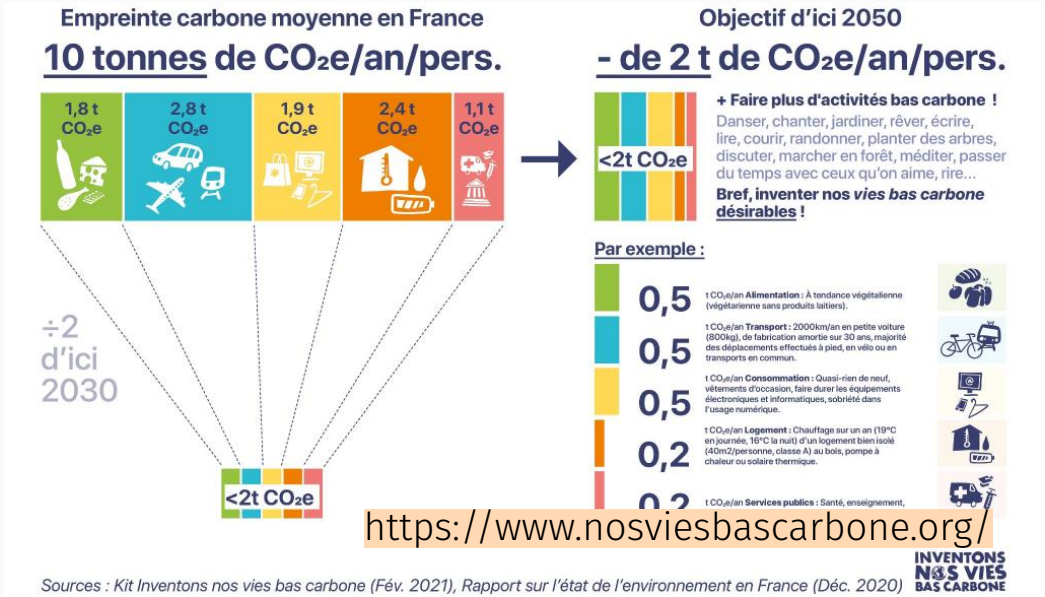

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~~Several~~ scenarios on the table

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