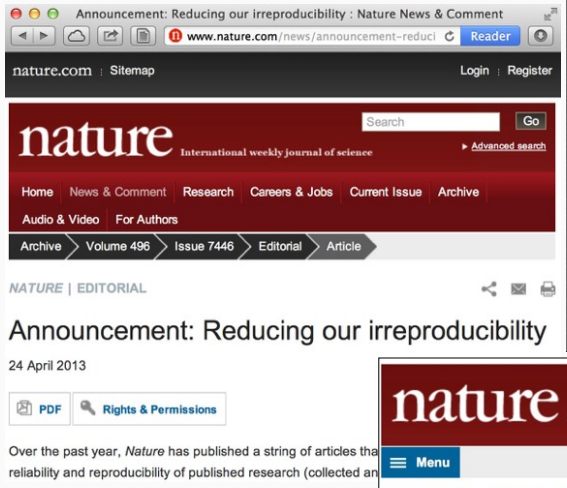
Reproducibility Crisis and Open Science

Arnaud Legrand
Univ. Grenoble Alpes, CNRS, Inria

Inria Alumni: Science Ouverte, November 2019

Public Evidence for a Lack of Reproducibility

- J.P. Ioannidis. *Why Most Published Research Findings Are False* PLoS Med. 2005.
- *Lies, Damned Lies, and Medical Science*, The Atlantic. Nov, 2010
- *Reproducibility: A tragedy of errors*, Nature, Feb 2016.
- Steen RG, Retractions in the scientific literature: is the incidence of research fraud increasing?. J. Med. Ethics 37, 2011



Courtesy V. Stodden, SC, 2015

Scientific Misconduct ? What are the Consequences ?

The Duke University scandal with scientific misconduct on lung cancer

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

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

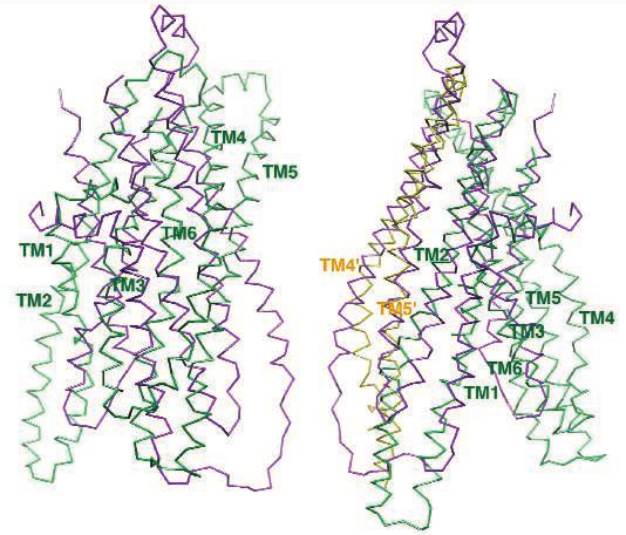
The Duke researchers continued to publish papers on their genomic signatures in prestigious journals. Meanwhile, they started three trials using the work to decide which drugs to give patients.

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

Bad science is deleterious

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

Unfortunate Mistakes



Geoffrey Chang (Scripps, UCSD) works on crystalography and studies the structure of cell membrane proteins.
He specialized in structures of multidrug resistant transporter proteins in bacteria: MsbA de Escheria Choli (Science, 2001), Vibrio cholera (Mol. Biology, 2003), Salmonella typhimurium (Science, 2005)

2006: Inconsistencies reveal a programming mistake

> *a homemade data-analysis program had flipped two columns of data, inverting the electron-density map from which his team had derived the protein structure.*

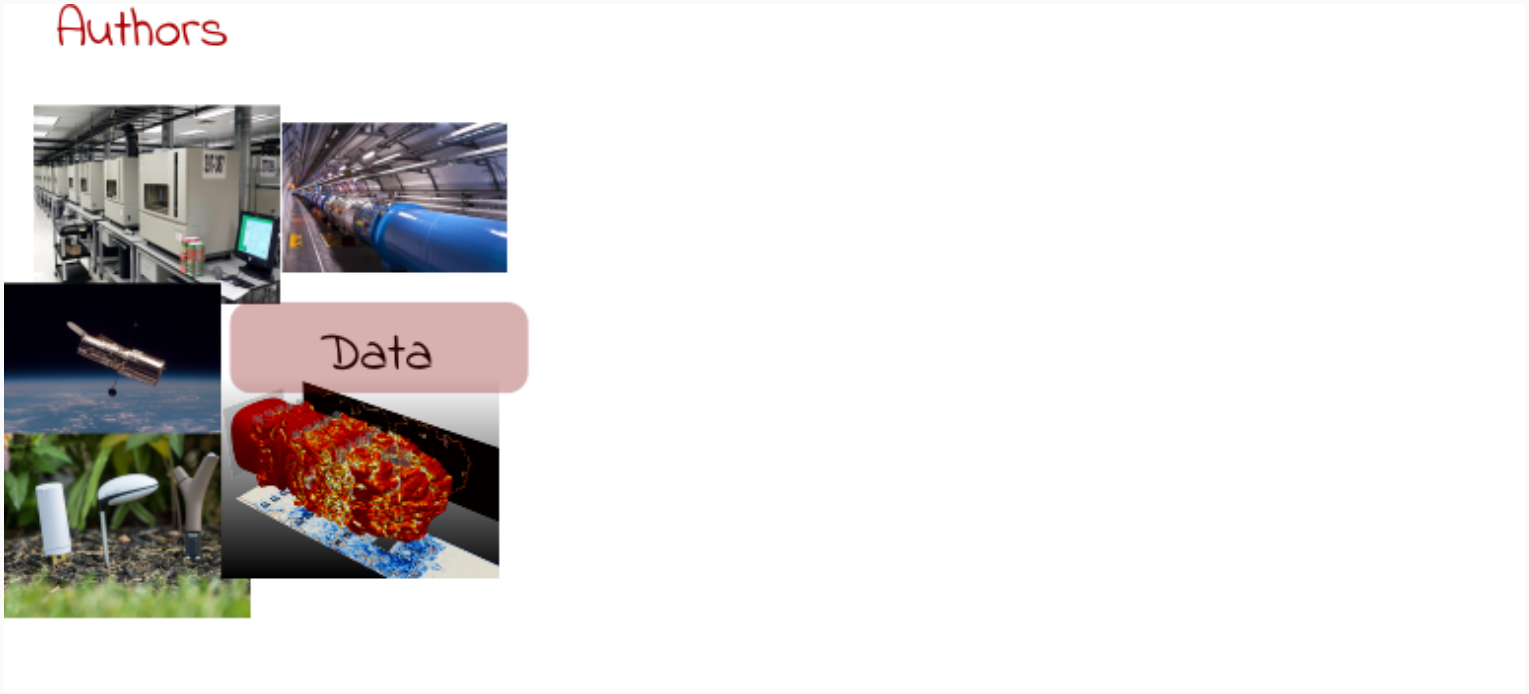
5 retractations that motivate improved software engineering practices in computational biology

Different Reproducibility Concerns

Social Sciences, Oncology methodology, statistics (p-hacking, HARKing)

Genomics software engineering, computational reproducibility, provenance

Computational fluid dynamics numerical issues



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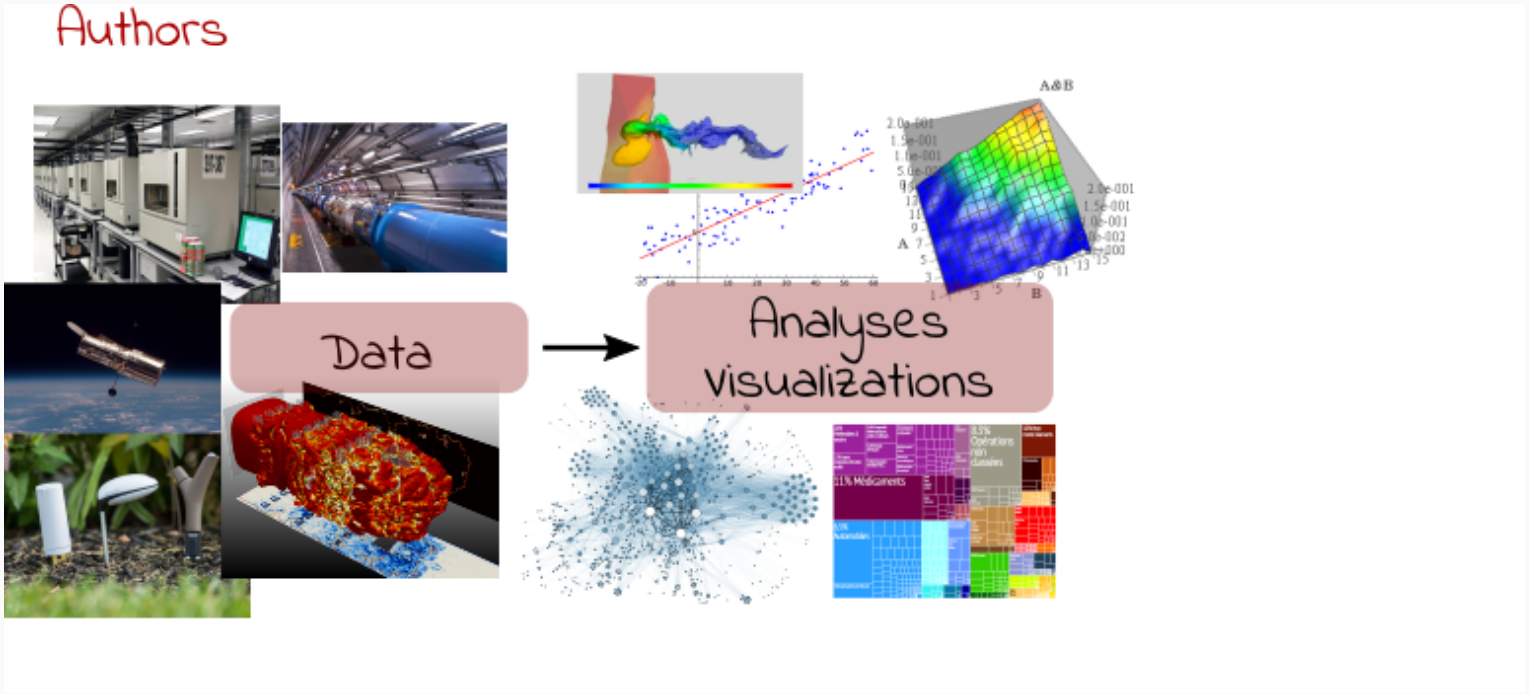

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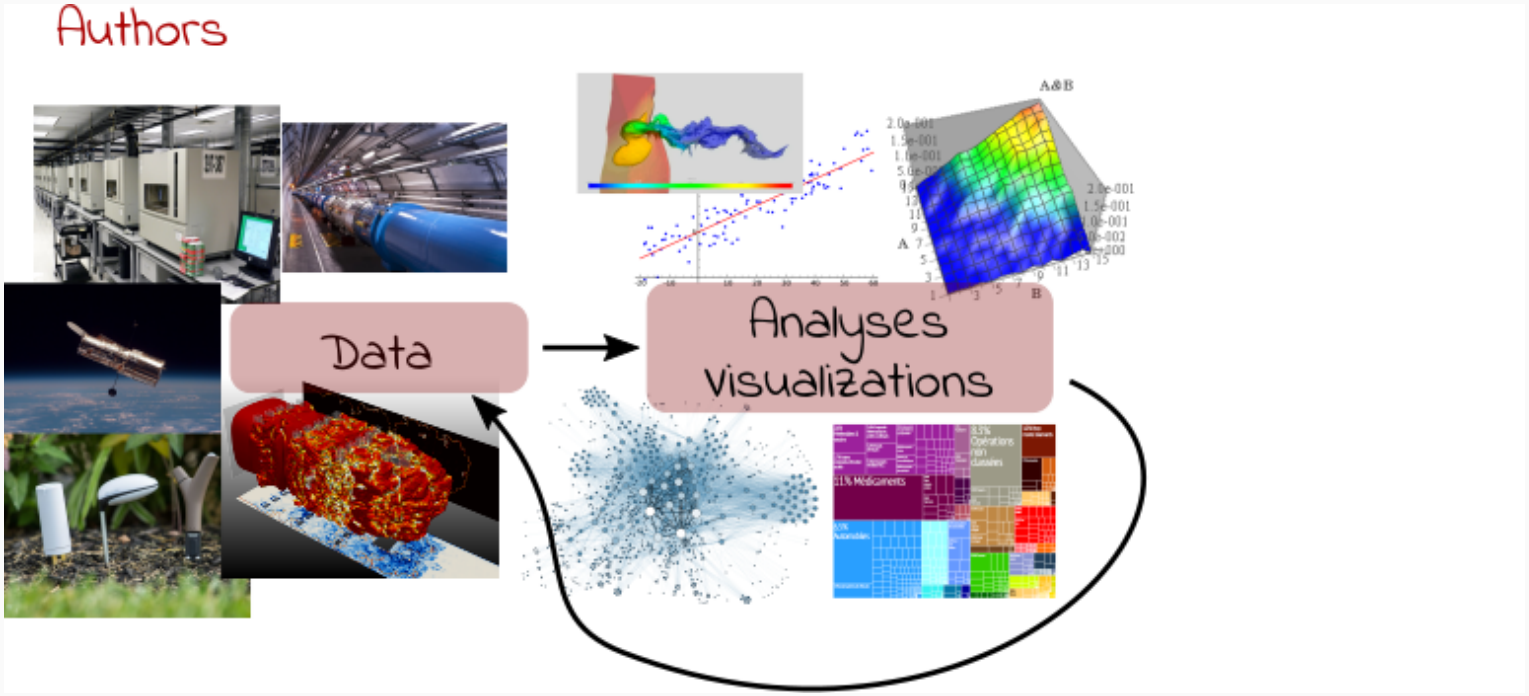

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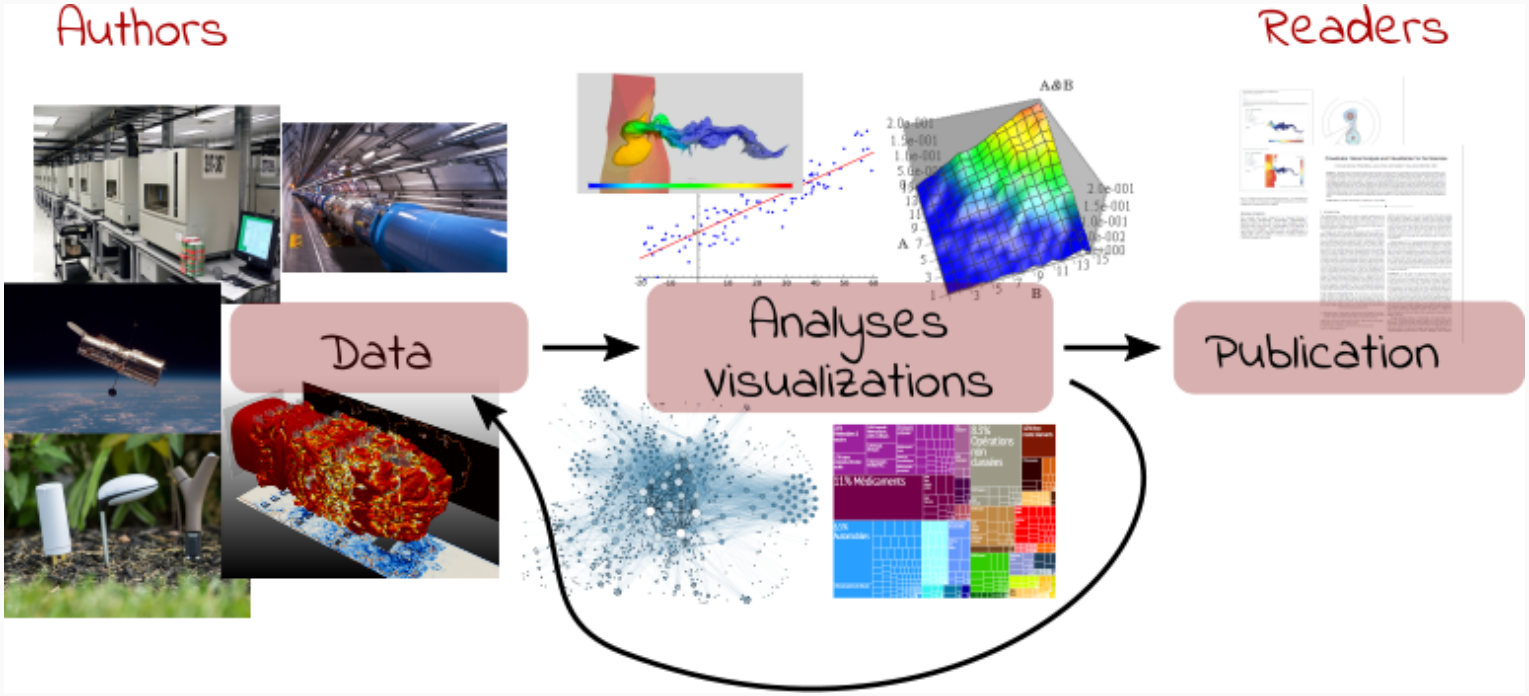

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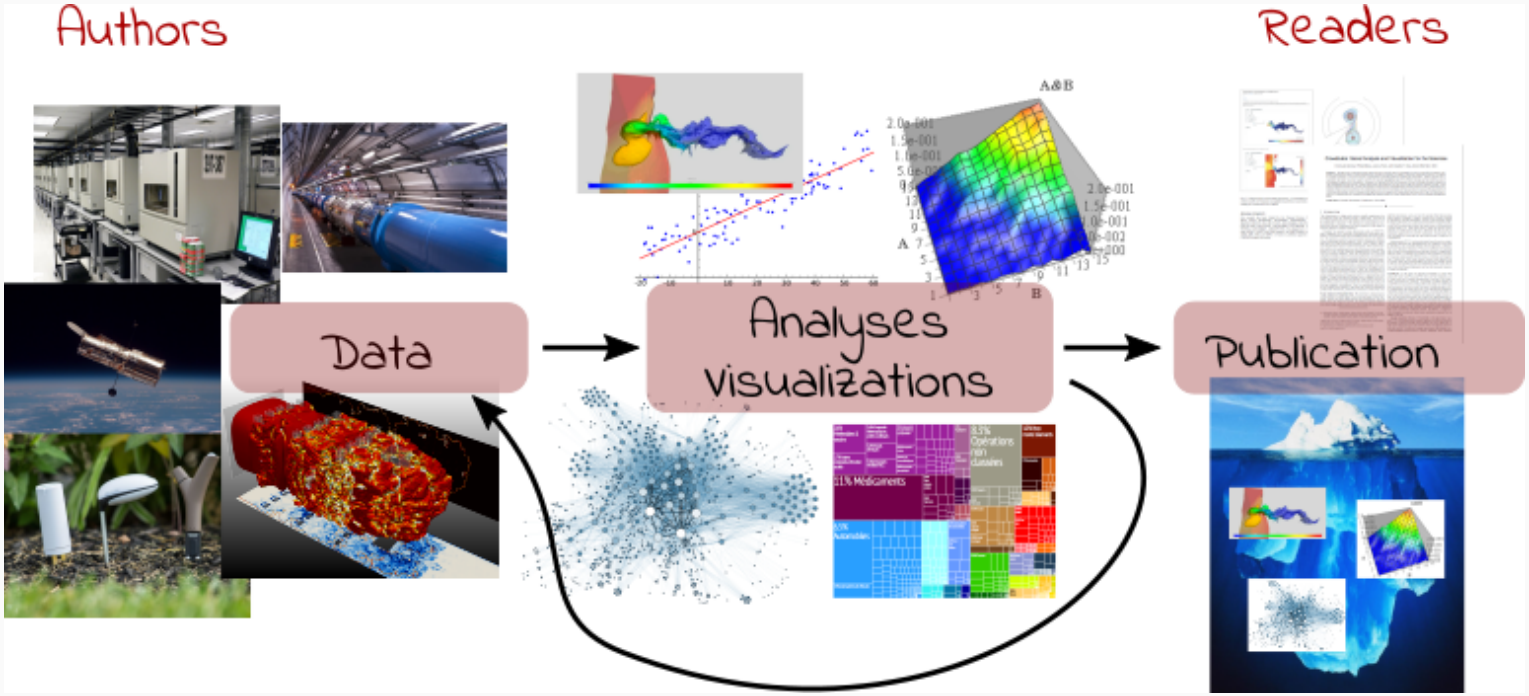

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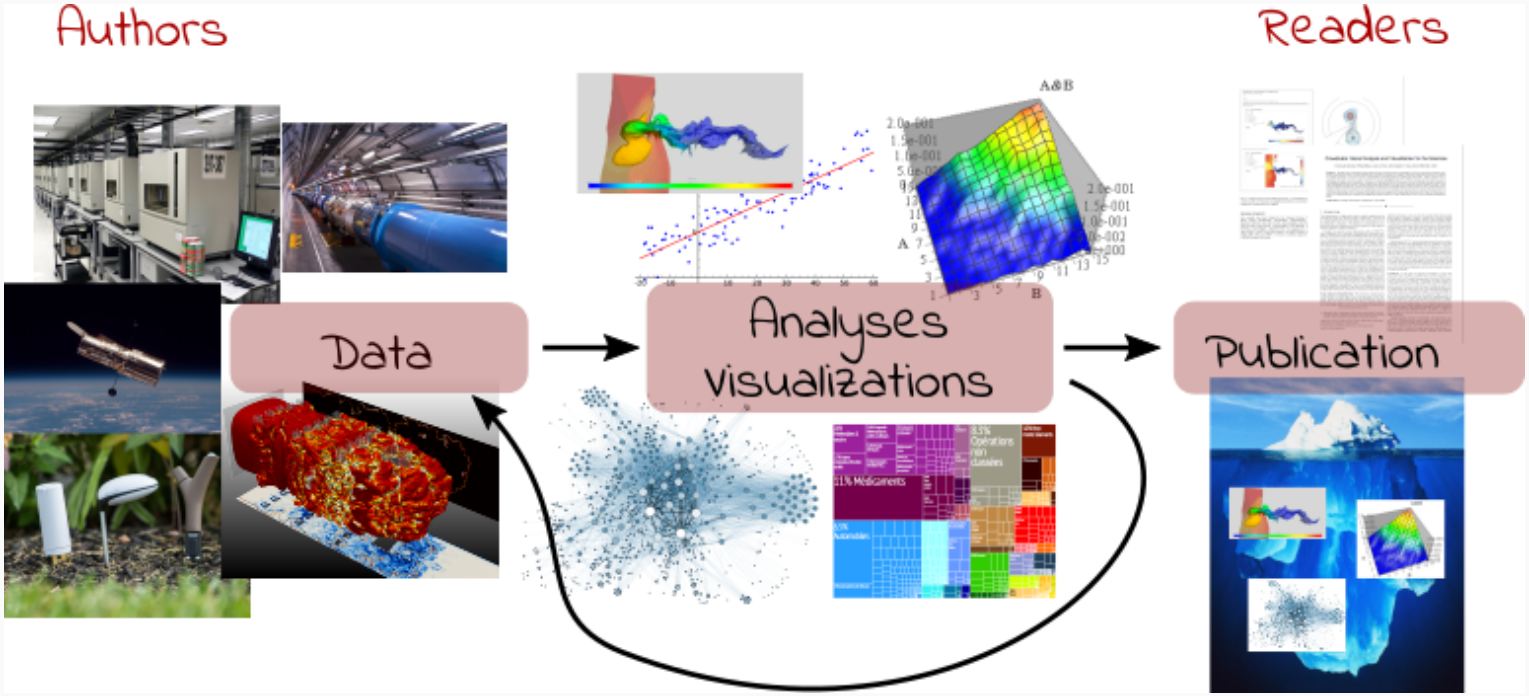
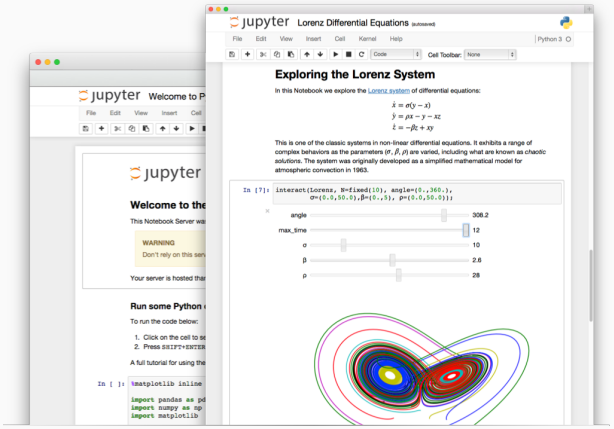


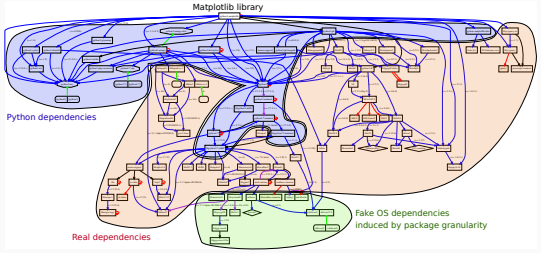
Reproducible Research = Bridging the Gap by working Transparently

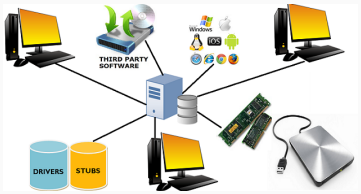
Existing Tools, Emerging Standards

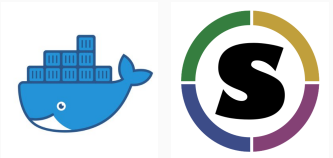
Notebooks and workflows



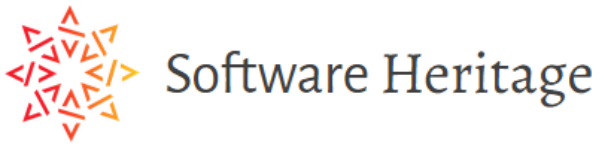
Software environments







Sharing platforms



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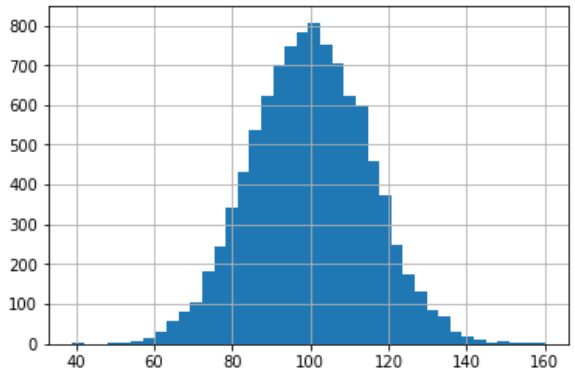

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jupyter example_pi (autosaved)

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Code CellToolbar

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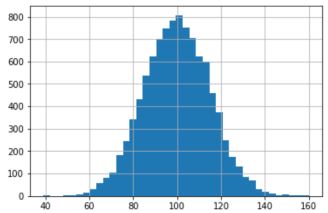

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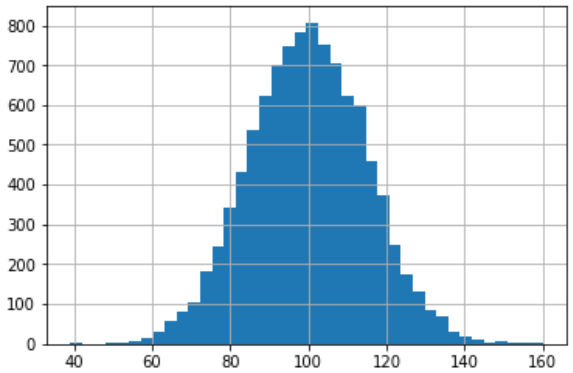

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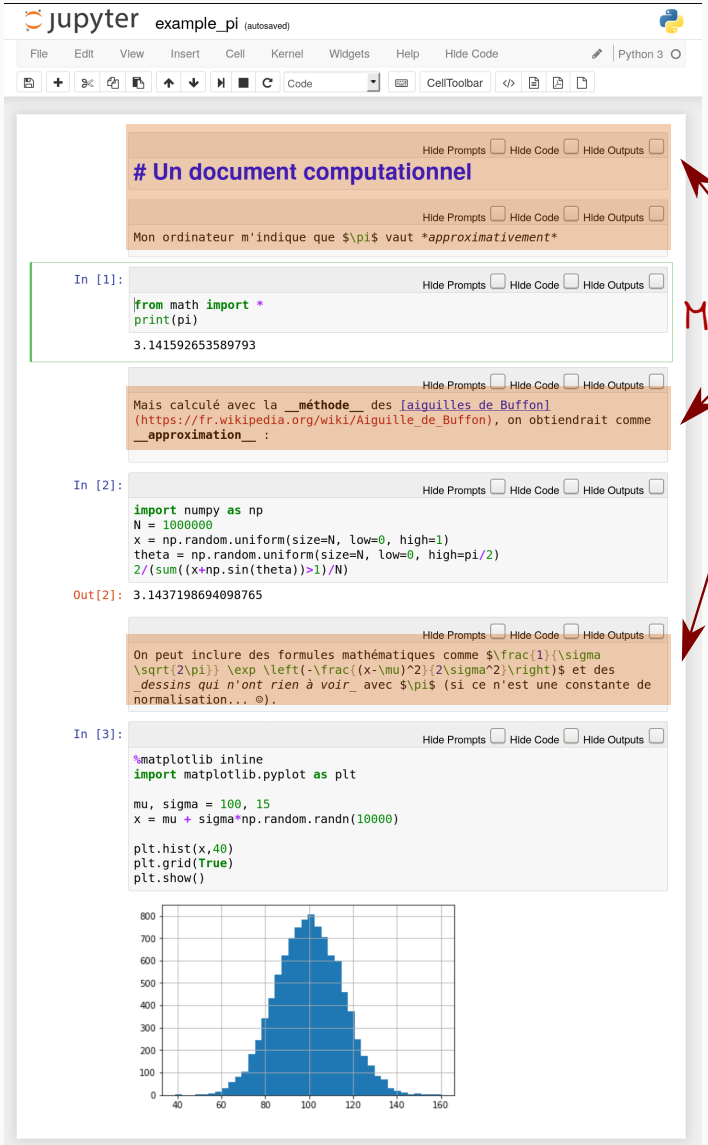

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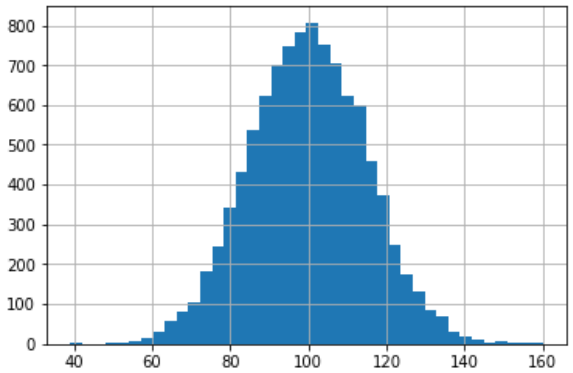

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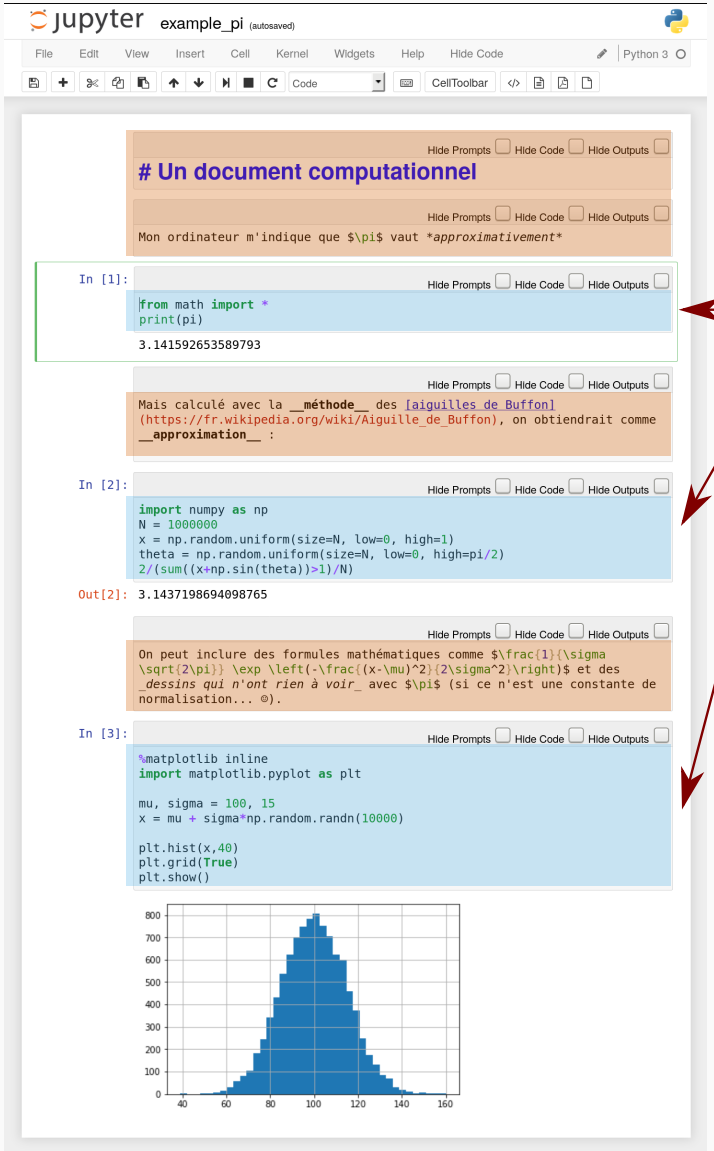

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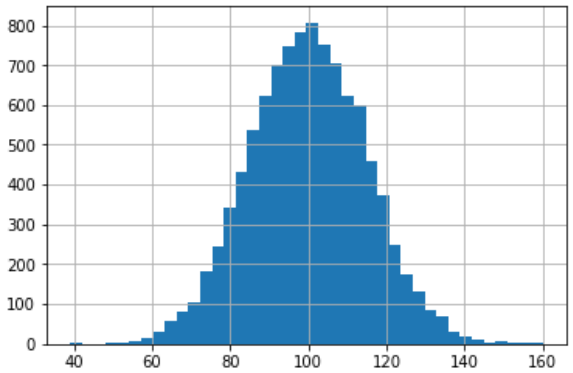

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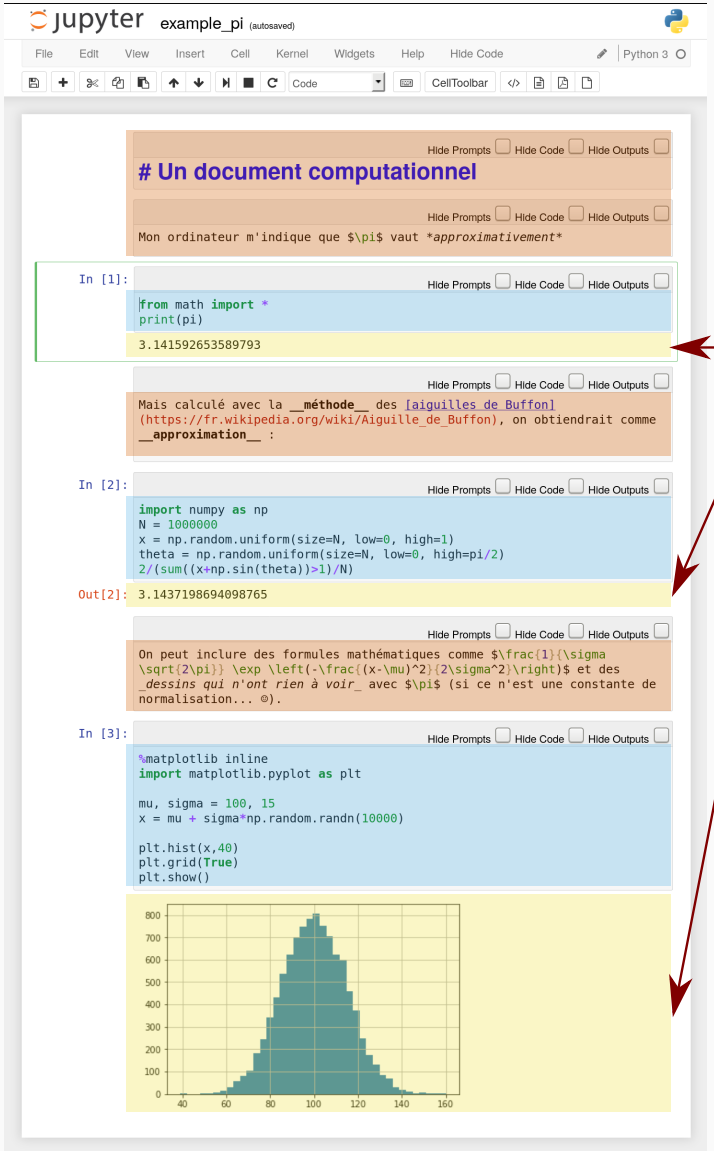

Résultats

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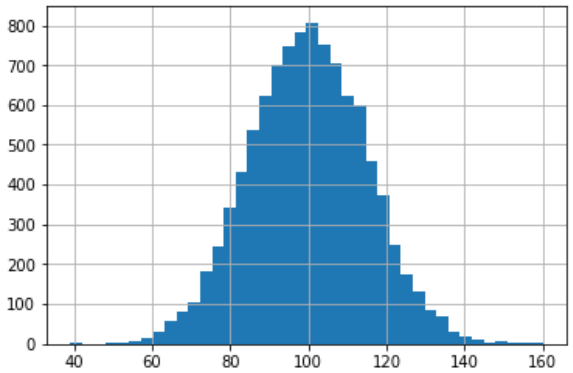

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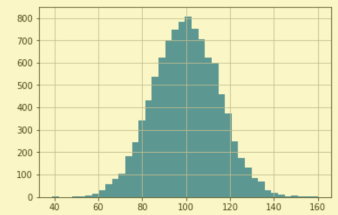

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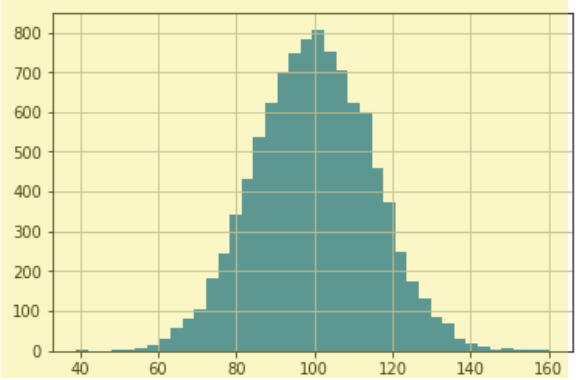

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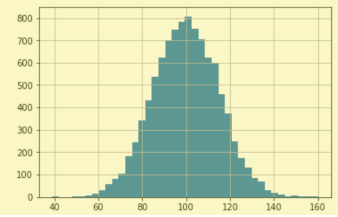

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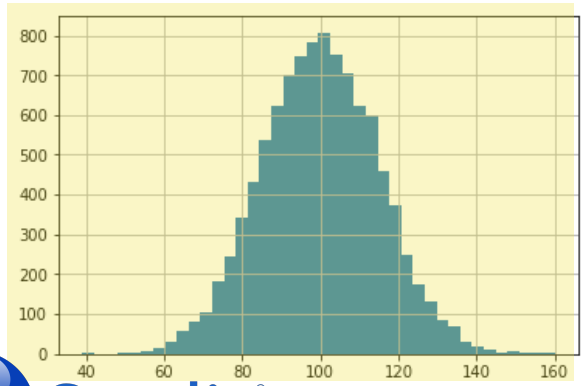
On peut inclure des formules mathématiques comme $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ et des *dessins qui n'ont rien à voir* avec π (si ce n'est une constante de normalisation... ☺).



Tool 2: Fighting Software Environments Nightmare

What is hiding behind a simple

```
1 import matplotlib
```

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

Tool 2: Fighting Software Environments Nightmare

What is hiding behind a simple

```
1 import matplotlib
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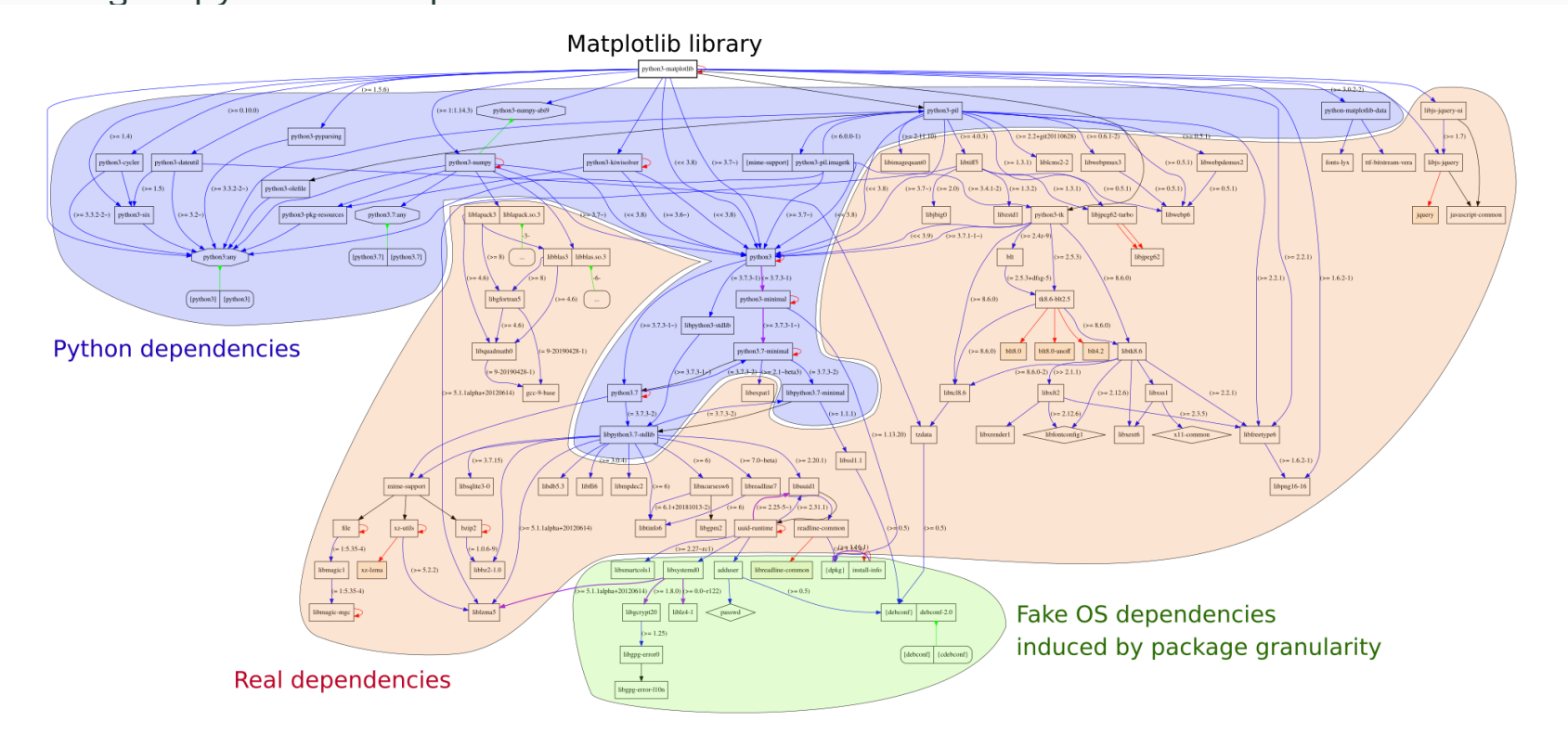
`Package: python3-matplotlib`



Tool 2: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

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

```
3
3.3333333333333335
```

Tool 2: Fighting Software Environments Nightmare

Python and its rapidly evolving environment

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

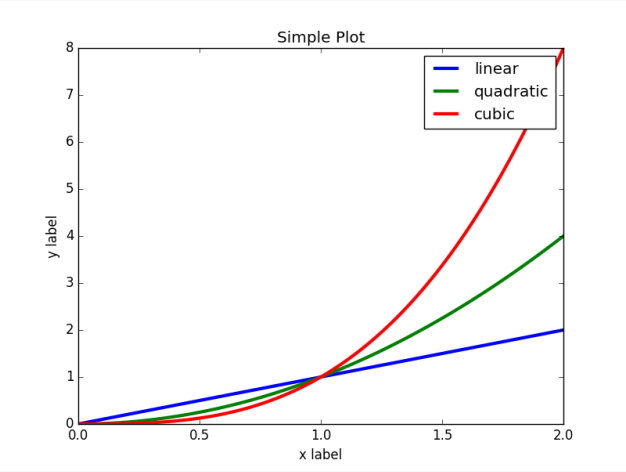

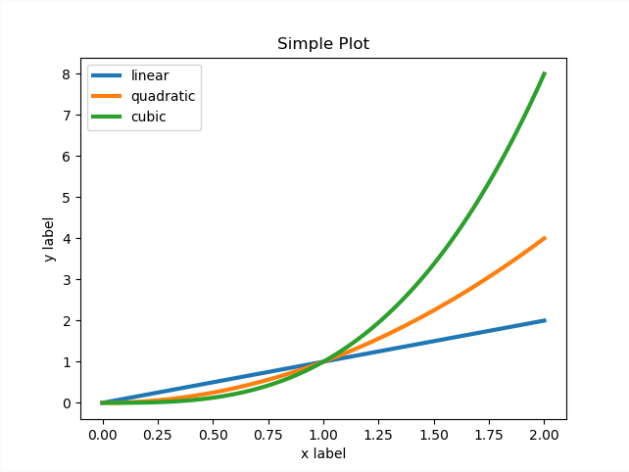

Tool 2: Fighting Software Environments Nightmare

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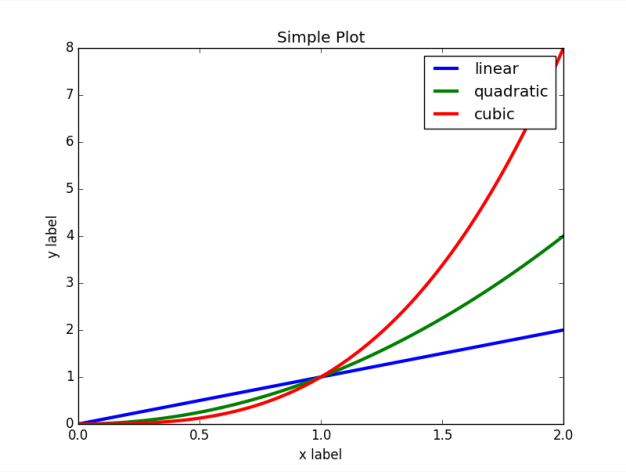

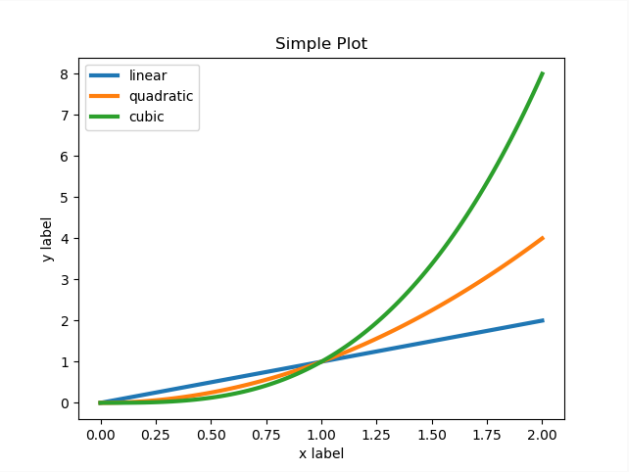

Cortical Thickness Measurements (PLOS ONE, June 2012): *FreeSurfer: differences were found between the Mac and HP workstations and between Mac OSX 10.5 and OSX 10.6.*

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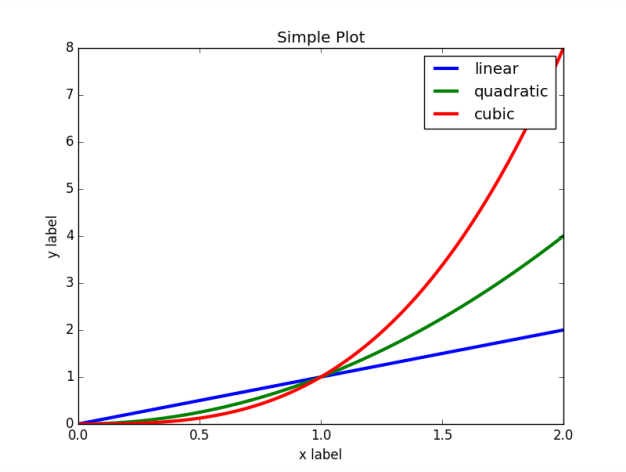

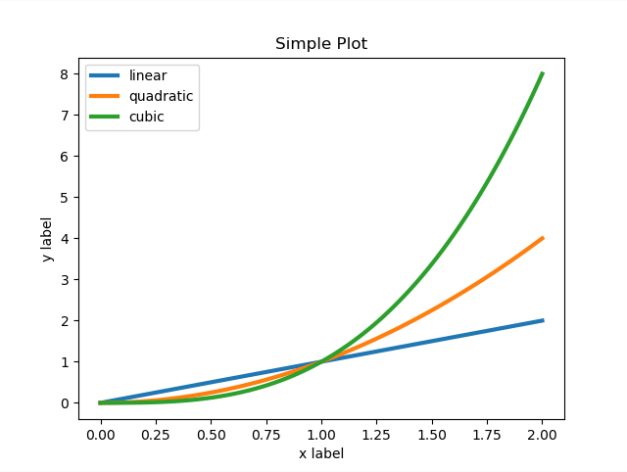

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ReproZip

Guix

Tool 3: Fighting Information Loss with Archives

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

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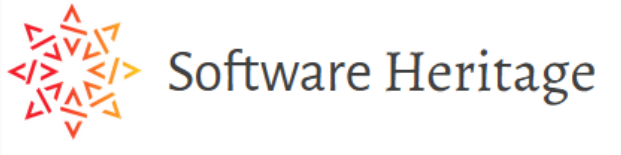
Article archives 

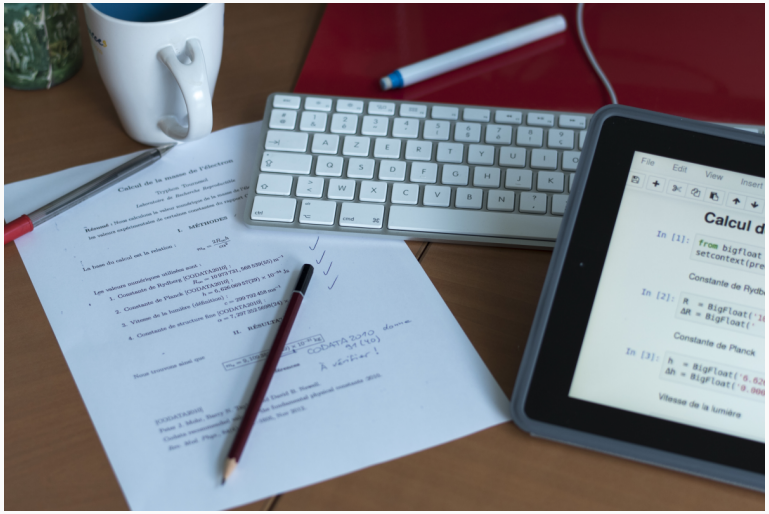
Data archives 

Software Archive 

 or  = awesome collaborations $\neq$ archive

Changing Research Practices

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



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

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

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

Changing Publishing Practices

Artifact evaluation and ACM badges

Major conferences

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

Joelle Pineau @ NeurIPS'18

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

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

Reproducible Research = Rigor and Transparency

To err is human: RR will not prevent errors nor fraud. It will help though

Good research requires time and resources

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

Perspectives and Opportunities

Transparency is not new. Interoperability and Reusability is newer

- This leads to fast and tremendous progress (e.g., Deep Learning)
- How Reusable is really Data and Software ?
  - Often specific, often impossible to customize despite openness
- Need for better *norms* ... but beware of brutal transitions
  - Acknowledge different kind of contributions (novelty vs. quality)
  - Independent experts and certification agencies
  - Embrace uncertainty

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Lack of reproducibility is mostly linked to statistics and computers

- Computer Science has no well-defined empirical practices yet
  - What can we expect from an experiment in terms of precision/representativeness/perenniality ?
- **Prepare the Future:** Toward literate experimentation?
  - Reuse, reuse, reuse!
  - Shared and controled testbeds (e.g., Grid'5000/SILECS)
  - How to share Experiments ?