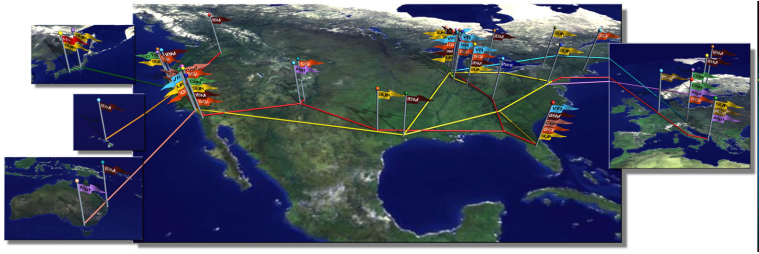
Reproducible Research, Open Science, Open Data, ...
Why ? Who ? How ?

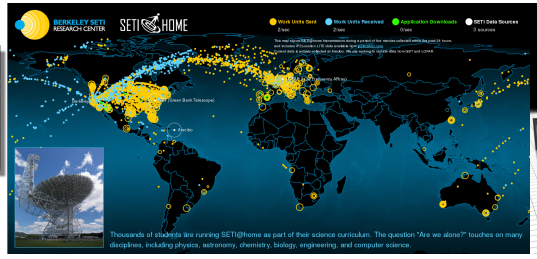
Arnaud Legrand
CNRS, Inria, University of Grenoble

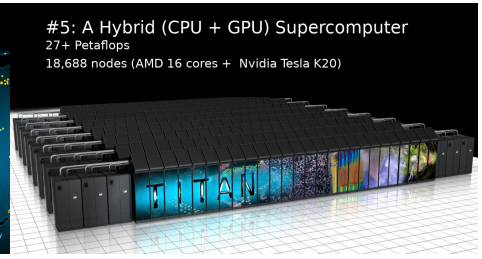
May 23rd, 2018 – Rennes, Inria DGD-T days

Who am I?

Application Domain Large scale computing infrastructures







Research Themes

- Optimization (scheduling, game theory)
- Performance Evaluation (modeling, simulation, analysis)

Proselytism in Scientific Methodology

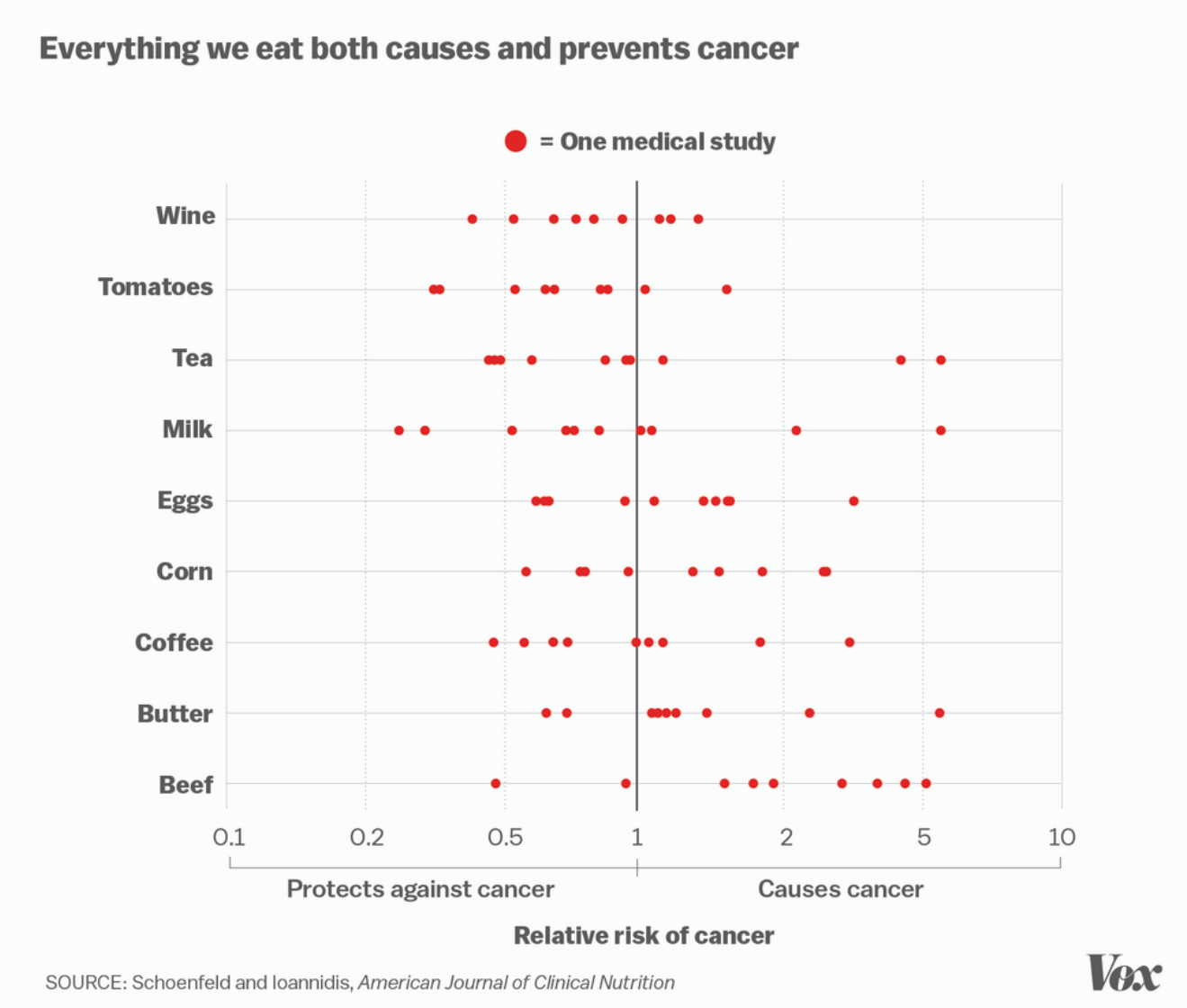
- Reproducible Research/Open Science
- Design of Experiments

Outline

Inconsistencies

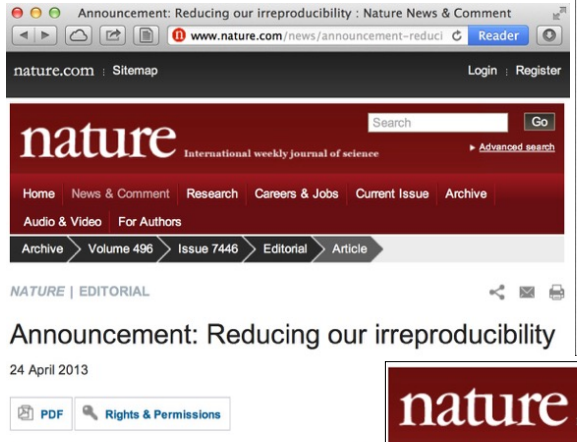
Is everything we eat associated with cancer? A systematic cookbook review, Schoenfeld and Ioannidis, *Amer. Jour. of Clinical Nutrition*, 2013.

Inconsistencies



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



Courtesy V. Stodden, SC, 2015

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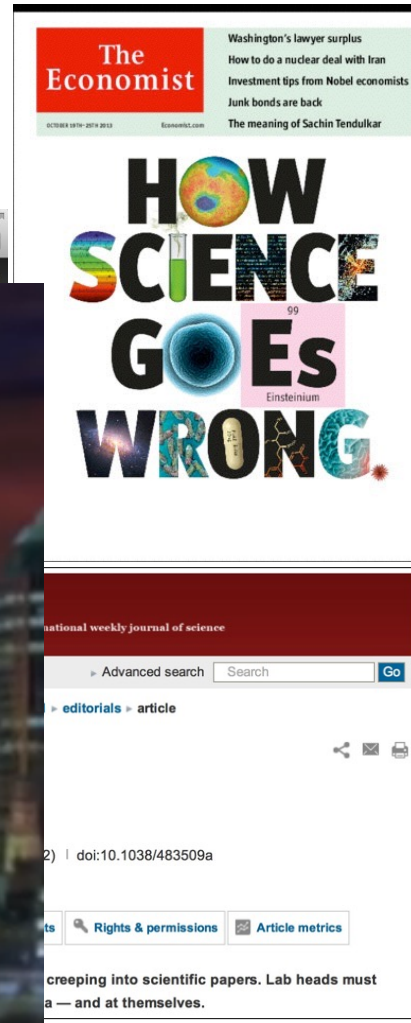
Last Week Tonight with John Oliver: Scientific Studies (HBO), May 2016



Courtesy V. Stodden, SC, 2015

Austerity in Fiscal Policy

2010 *"gross debt [..] exceeding 90 percent of the economy has a significant negative effect on economic growth"*

– Reinhart et Rogoff: Growth in a Time of Debt

2013 *While using RR's working spreadsheet, we identified coding errors, selective exclusion of available data, and unconventional weighting of summary statistics.*

– Herndon, Ash and Pollin

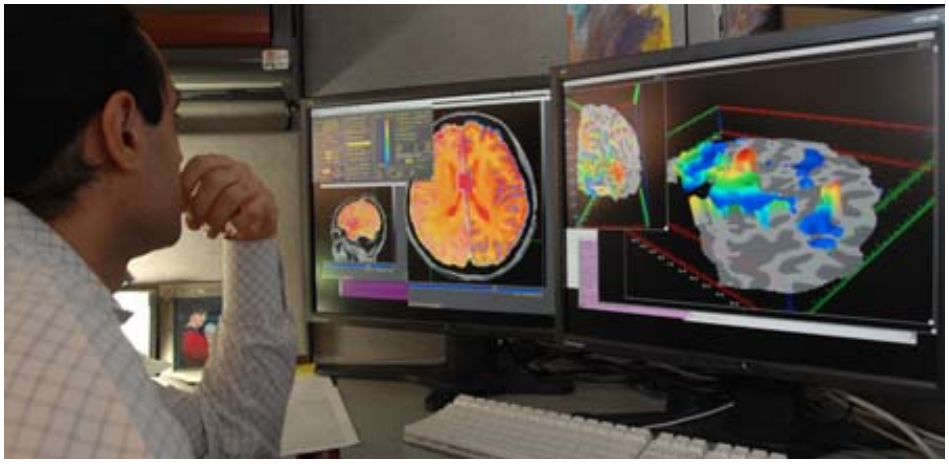
combining data across centuries, exchange rate regimes, public and private debt, and debt denominated in foreign currency as well as domestic currency

– Wray

For 3 years, austerity was not presented as an option but as a necessity.

Yet, a scientific debate has at least been possible.

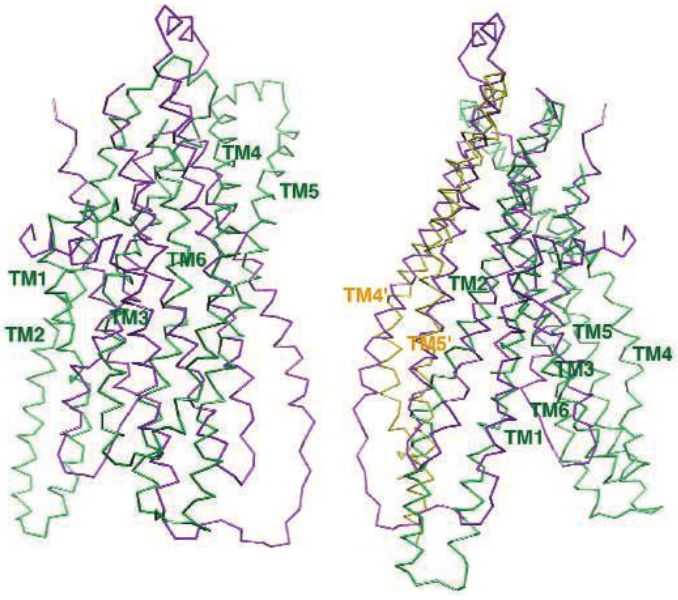
FRMI



- 2010: Bennett et al. and the dead salmon ☺
- 2016: Eklund, Nichols, and Knutsson. A bug in fmri software could invalidate 15 years of brain research (*40,000 articles*, although it is a bit more subtle than this).
- 2016: Nichols. $\approx$ *3 600 articles may have to be revisited for confirmation.*

These article do not necessarily invalidate everything but force the community to improve their practice.

Geoffray Chang's incorrect protein structures



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

A Reproducibility Crisis? What are the Consequences ?

The Duke University scandal with scientific misconduct on lung cancer

- *Nature Medicine* - 12, 1294 - 1300 (2006) Genomic signatures to guide the use of chemotherapeutics, by Anil Potti and 16 other researchers from Duke University and University of South Florida
- 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

Well... Stronger and Stronger Consequences

A recent scandal In 2013, *Dong-Pyou Han*, a former assistant professor of biomedical sciences at Iowa State University was disgraced:

- Falsified blood results to make it appear as though a vaccine he was working on had exhibited anti-HIV activity
- Han and his team received $\approx$ \$19 million from NIH
- Retraction and resignation of university

Han was sentenced in 2015 to 57 months imprisonment for fabricating and falsifying data in HIV vaccine trials. He was also fined US \$7.2 million!

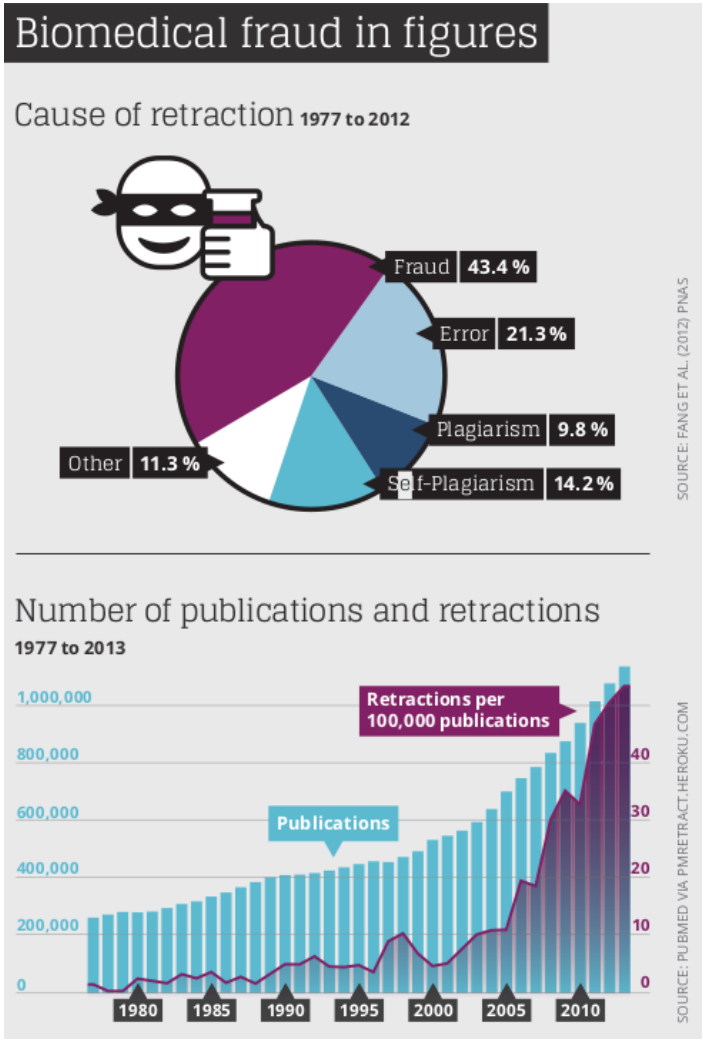
We should avoid witch-hunt

- August 5, 2014, Yoshiki Sasai (stem cell, considered for Nobel Prize) hanged in his laboratory at the RIKEN (Japan). Fraud suspicion...
- In 1986, a young postdoctoral fellow at MIT accused her director, Thereza Imanishi-Kari, of falsifying the results of a study published in Cell and co-signed by the Nobel laureate David Baltimore. [..] Declared guilty, Univ. presidency resignation, and finally cleared. This put the careers of two outstanding researchers on hold for ten years based on unfounded accusations.

Scientific fraud is bad but let's be careful Have a look at the wikipedia *list of academic scandals*.

Is Fraud a new phenomenon?

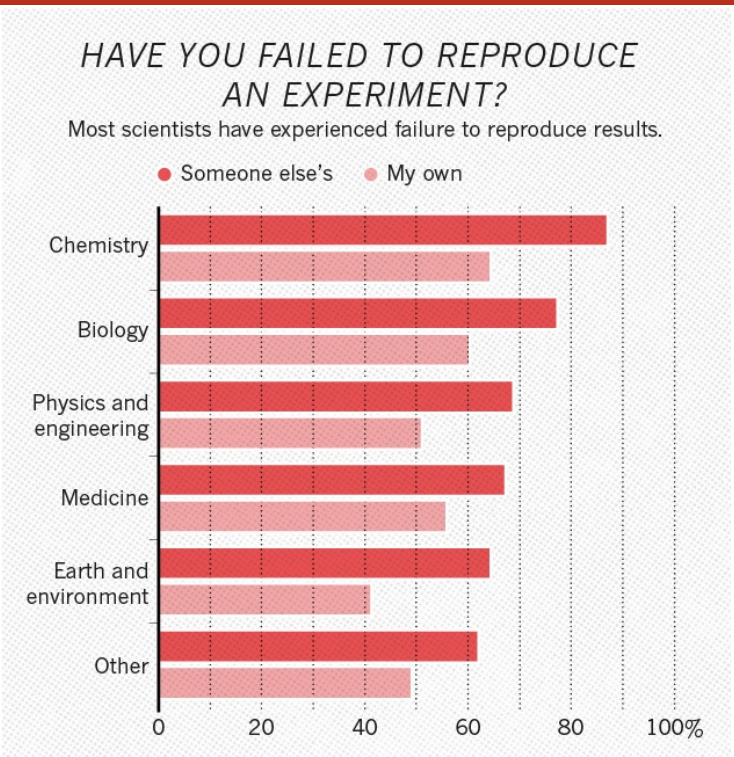
The Battle against Scientific Fraud in the CNRS International Magazine

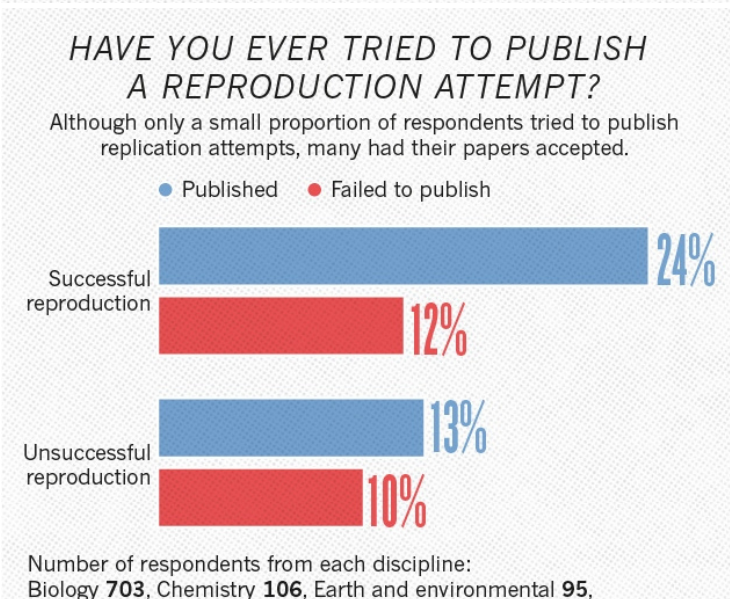


Galileo (data fabrication), Ptolemy (plagiarism), Mendel (data enhancement), Pasteur (rigorous but hided failures), ...

Is it only a matter of Fraud ?

Why are scientific studies so difficult to reproduce?





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: 1+ million articles per year!

Methodological or 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

Wrap-up

- Oncology : "*more than half studies published in prestigious journals cannot be reproduced in industrial labs*"
- Psychology : "*replicating a hundred of major articles: only one third of coherent results*"

Whistle blowers, sick institutions, broken system, ?..

No. Questionning previous work is part of the scientific process

Just like honesty, rigor and transparency. . .

Risks science credibility put into question. No more difference with crooks!

Outline

Computational science!

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

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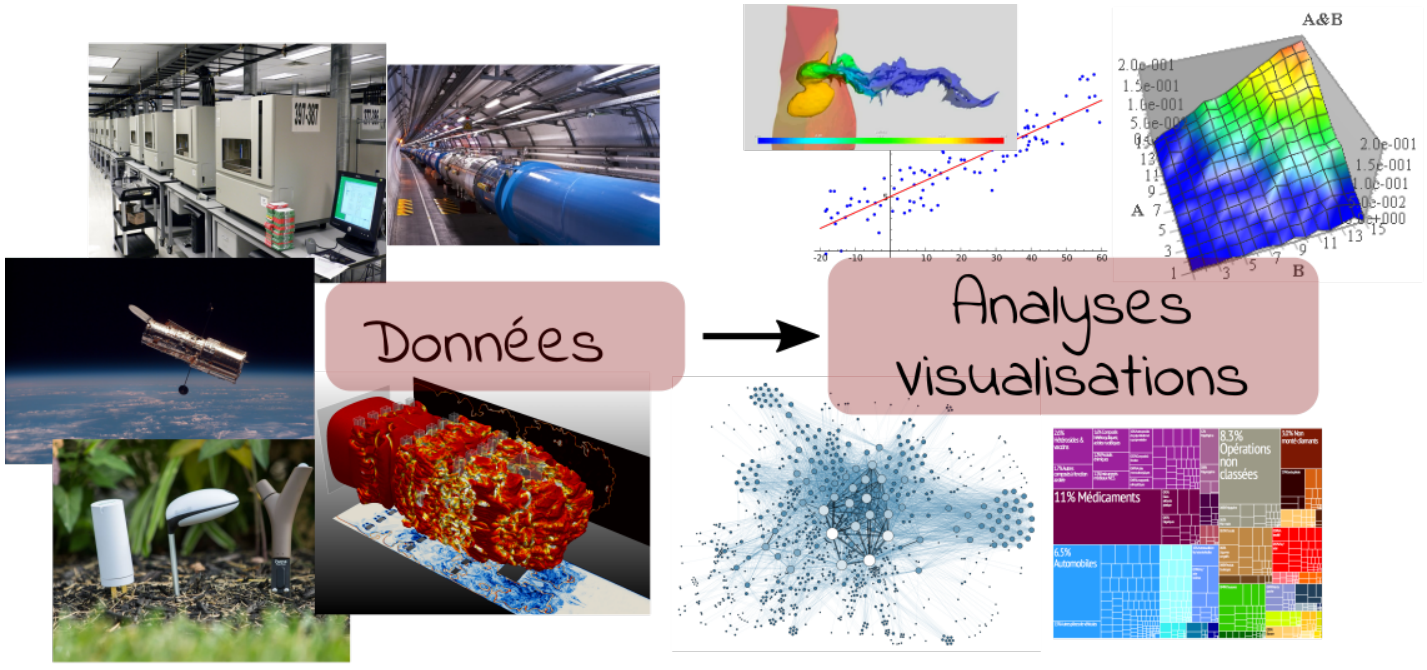

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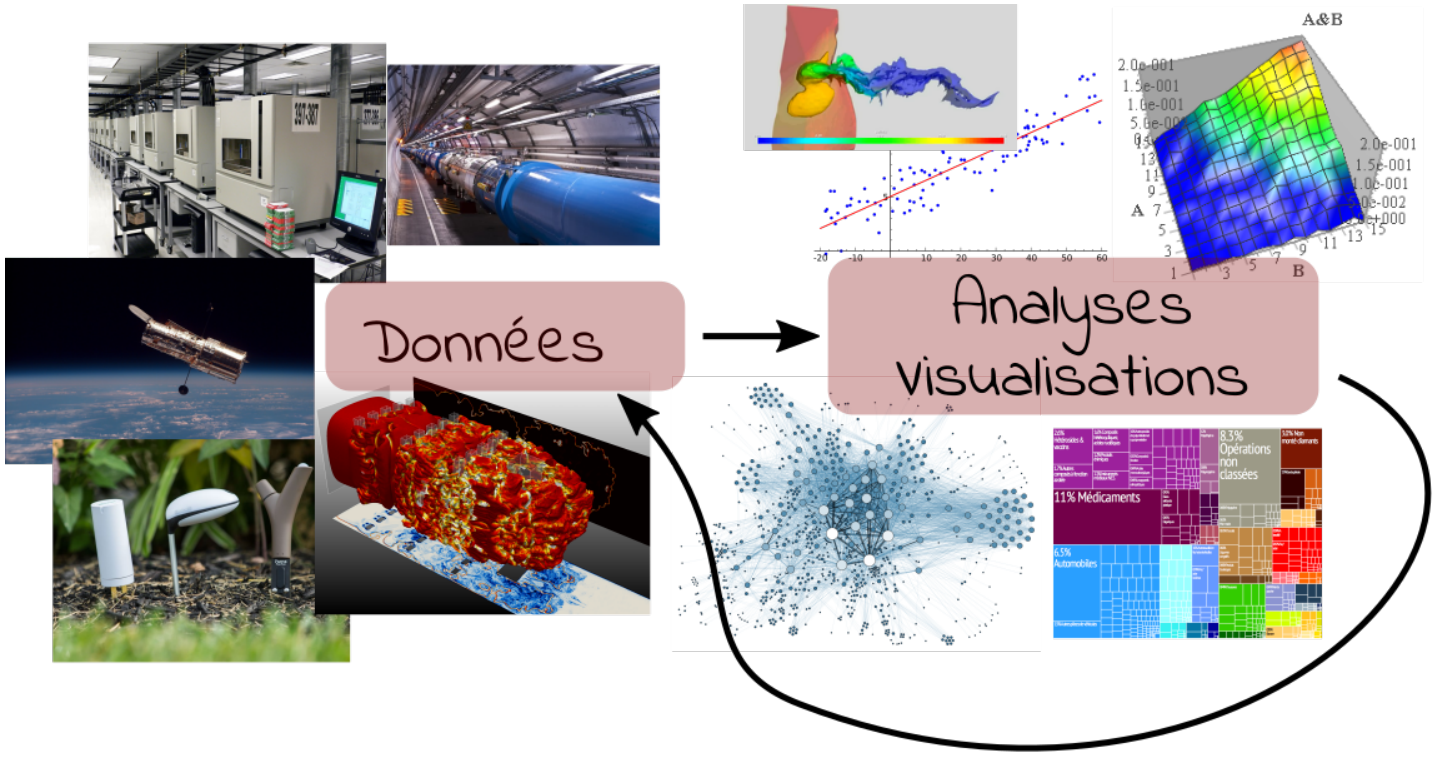

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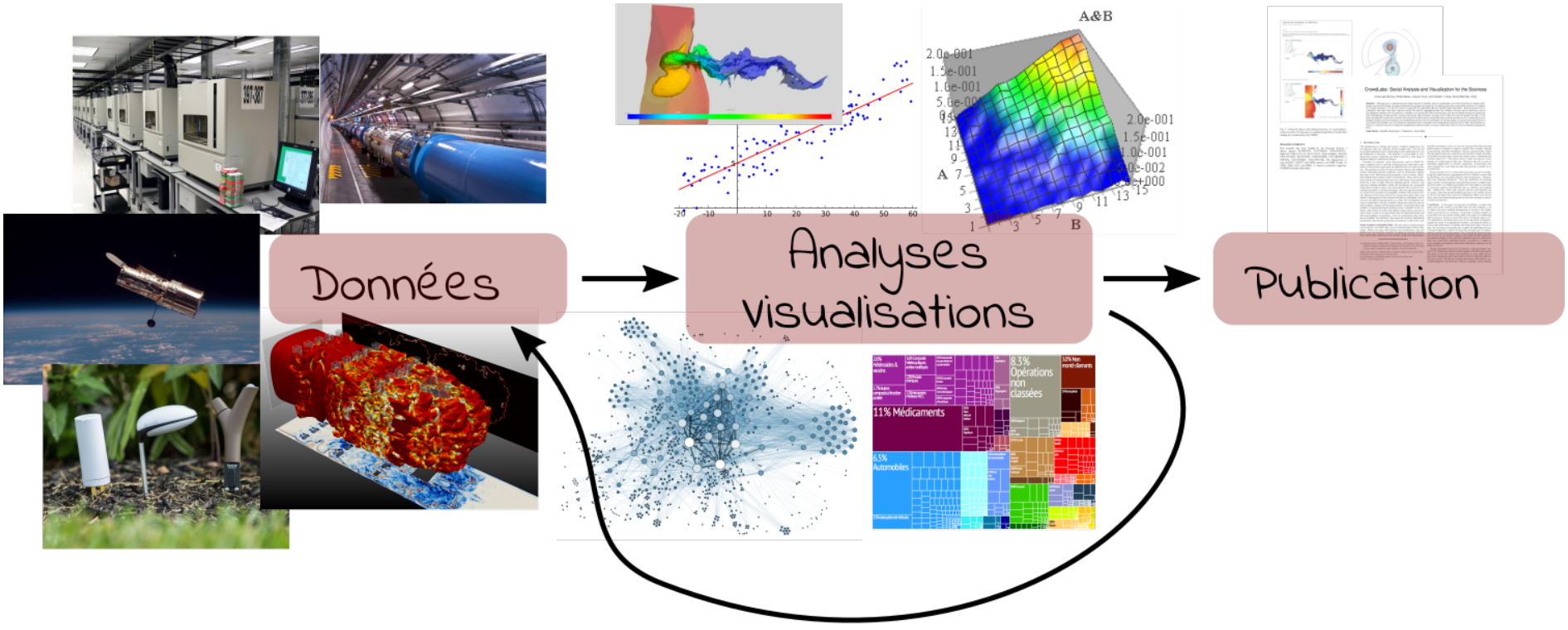

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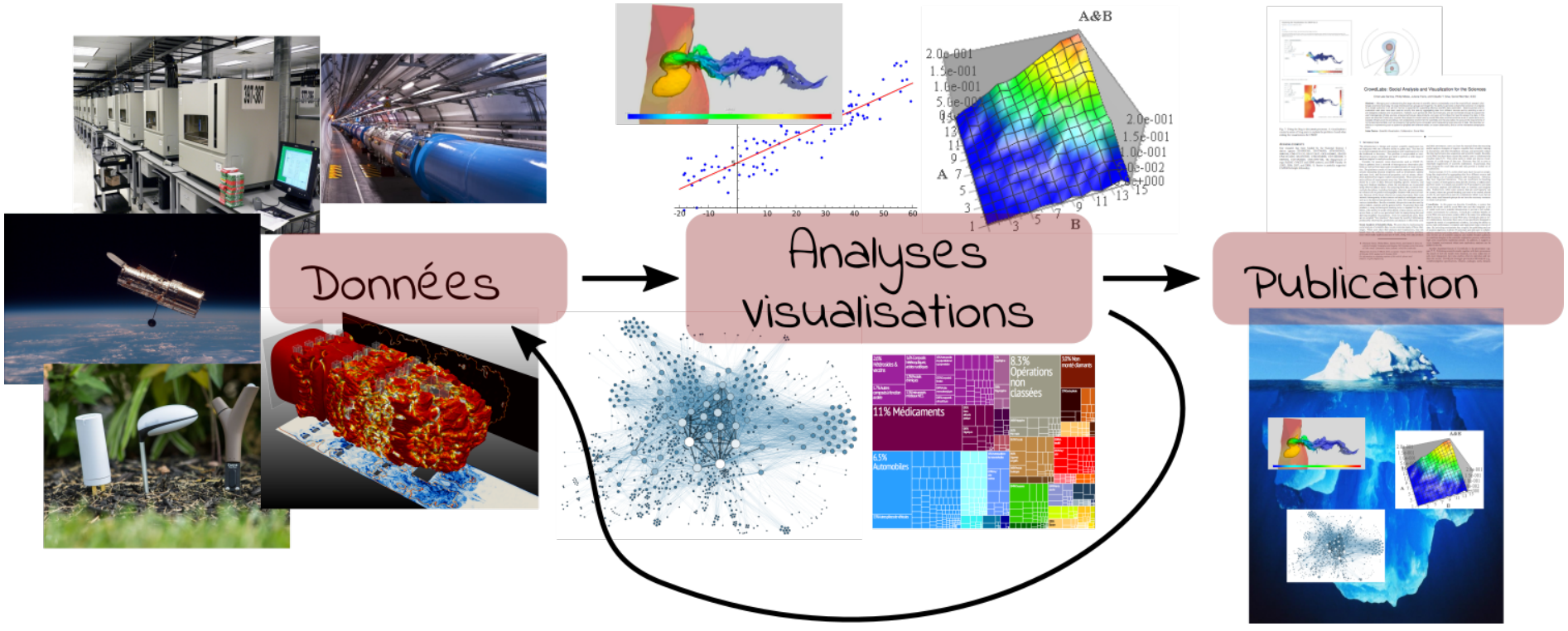

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Aren't Computers Good for Science ?

How computers broke science – and what we can do to fix it.

- Point and click
- Spreadsheets : programming and data manipulation mistakes
  - `Membrane-Associated Ring Finger (C3HC4) 1, E3 Ubiquitin Pro Ligase` → `MARCH1` → 2016-03-01 → 1456786800
  - `2310009E13` → 2.31E+19
- Complex software stacks : avoid proprietary software as much as possible
- Bugs : *Programming is difficult !*

All this is about Natural Sciences. Should we care ?

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

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

- Have a look at talk by Vladimir Voevodsky in 2014 at Princeton 🙂

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  Computer science is not more related to computers than Astronomy to telescopes

  – Dijkstra (mis-attributed)

Right, why should we care about computers? They are deterministic machines after all, right? 😉

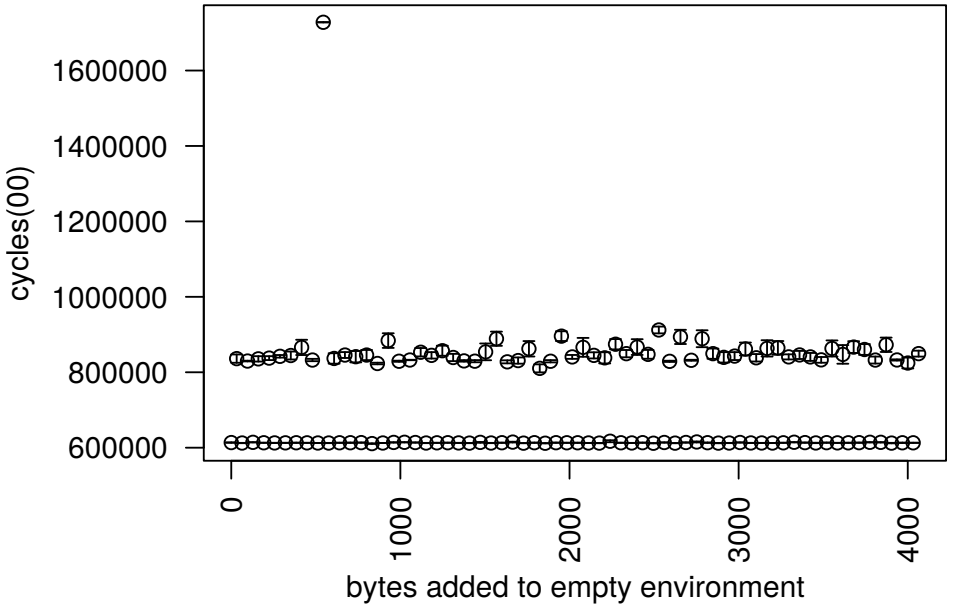
Model $\neq$ **Reality**. Although designed and built by human beings, computer systems are so complex that mistakes easily slip in...

Experimenting with computers

Machines are real!

Brendan Gregg: Shouting in the data center

Machines are complicated



Mytkowicz et al. Producing wrong data without doing anything obviously wrong!
ACM SIGPLAN Not. 44(3), March 2009

Our reality evolves!!! The hardware keeps evolving so most results on old platforms quickly become obsolete (although, we keep building on such results 😉).

- We need to regularly revisit and allow others to build on our work!

Computer performance ? Well, I design algorithms!

- "Real" problems are all NP-hard, Log-APX, etc.
- Real workload = ~~NP-completeness proof widgets~~, regularities and properties (difficult to formally state but that should be exploited)

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Image Processing: True horror stories, E. Meinhardt-Llopis, CANUM 2016

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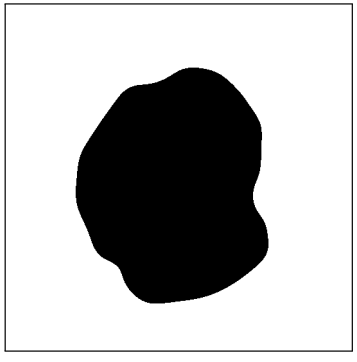
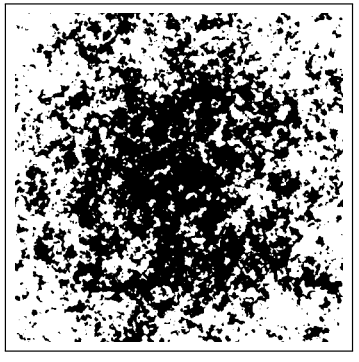




I design Machine Learning Algorithms

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".* – *Sandy Pentland (MIT)*

Every month in CACM, there is an article about the ethical consequences of Machine Learning on:

- Car driving, Autonomous guns, Law enforcement (risk assessment, predictive policing), ...

  It's Not the Algorithm, It's the Data (CACM, Feb. 2017)

- Advertising, Loan attribution, Selection at University, Organ transplant

Increasing society concern about fairness and transparency

All I care about is the algorithm output

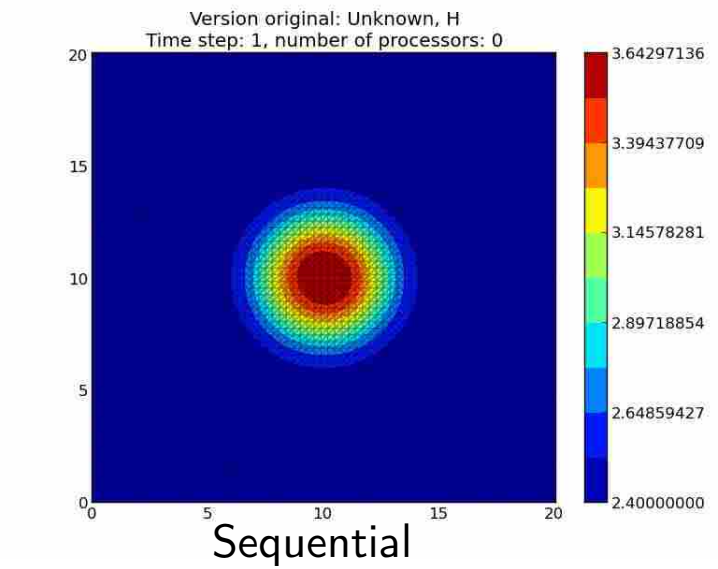
Did I mention we have parallel machines nowadays? 😉

Telemac2D: the simplest gouttedo simulation

The gouttedo test case

- 2D-simulation of a water drop fall in a square bassin
- Unknown: water depth for a 0.2 sec time step
- Triangular mesh: 8978 elements and 4624 nodes

Expected numerical reproducibility (time step = 1, 2, . . .)



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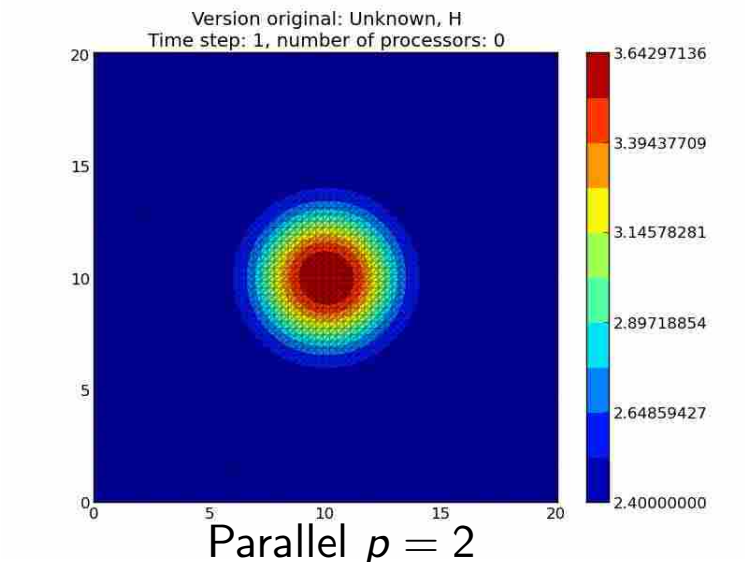

Parallel $p = 2$

Courtesy of P. Langlois and R. Nheili

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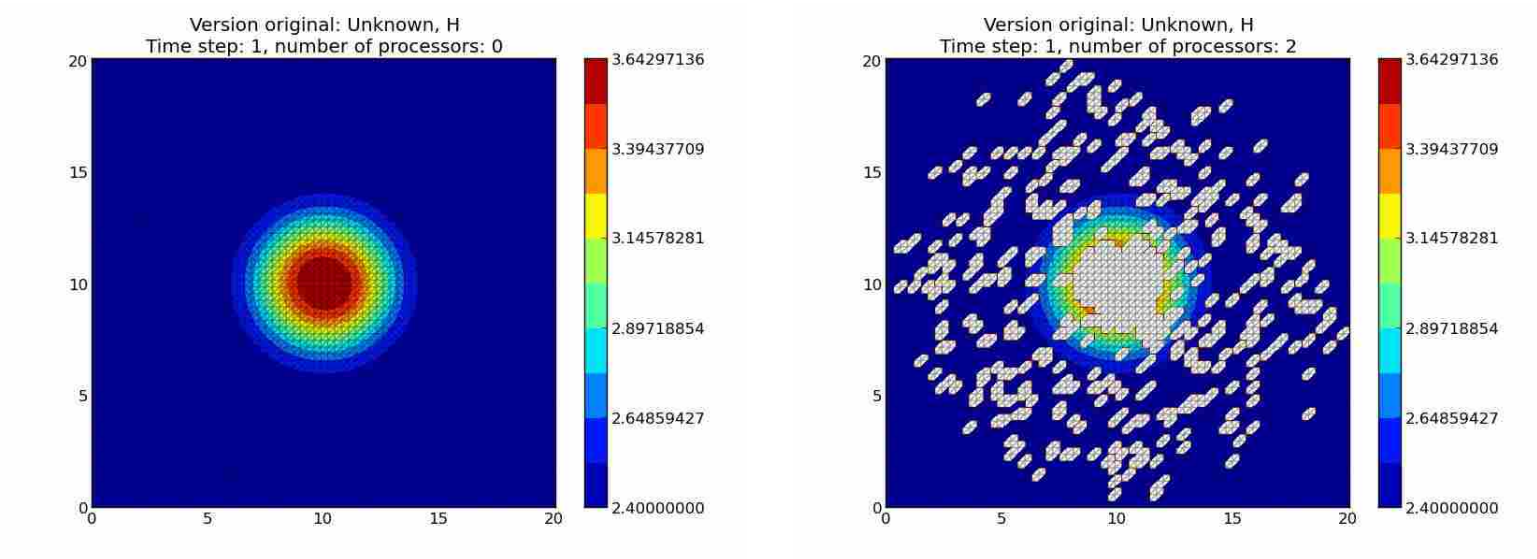
A white plot displays a non-reproducible value

Numerical reproducibility?

time step $= 1$



Sequential

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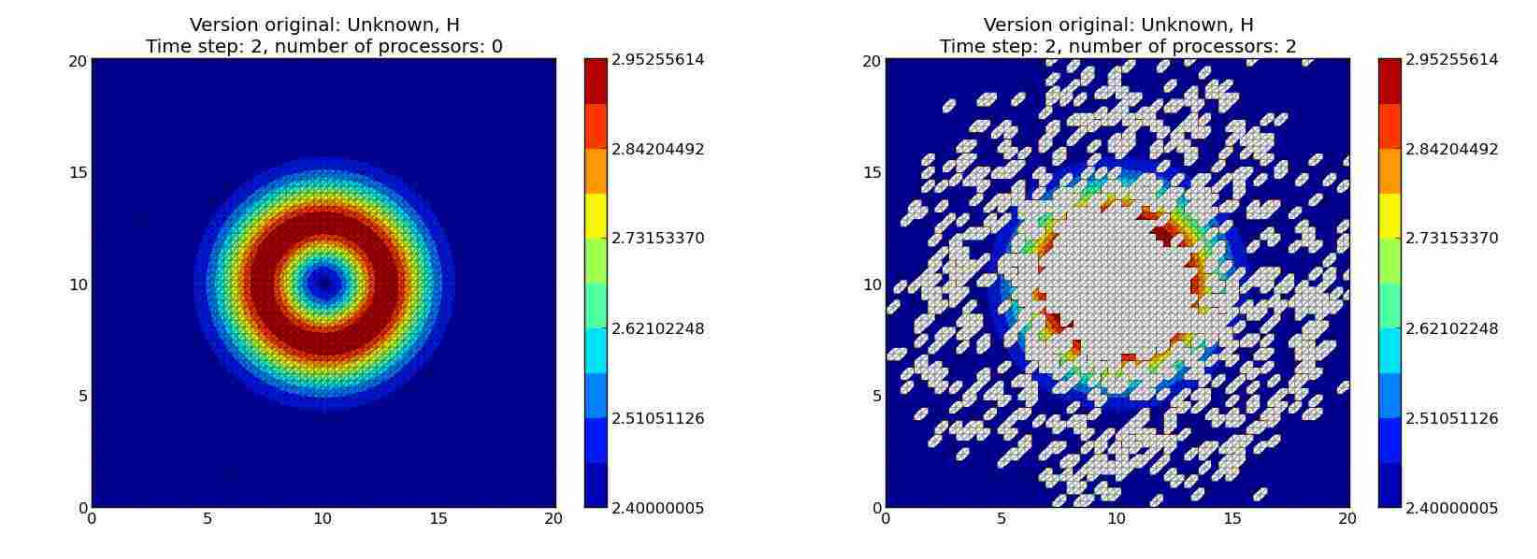
Numerical reproducibility?

time step = 2



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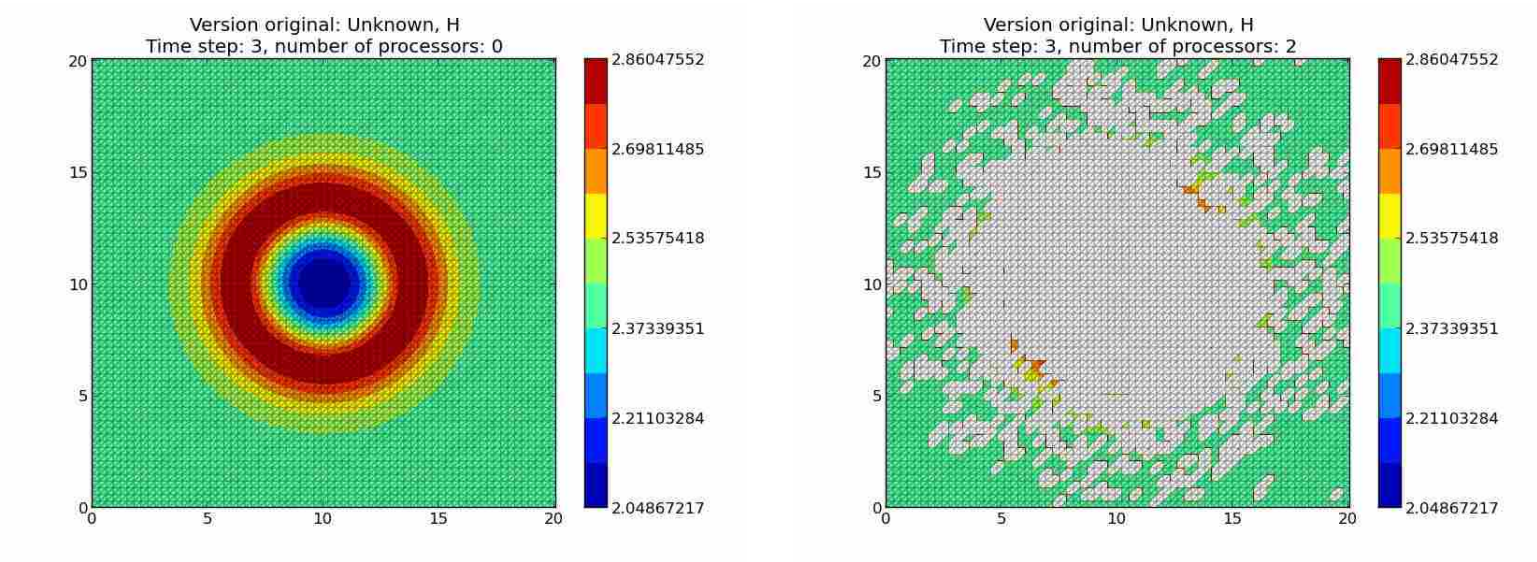
time step = 3



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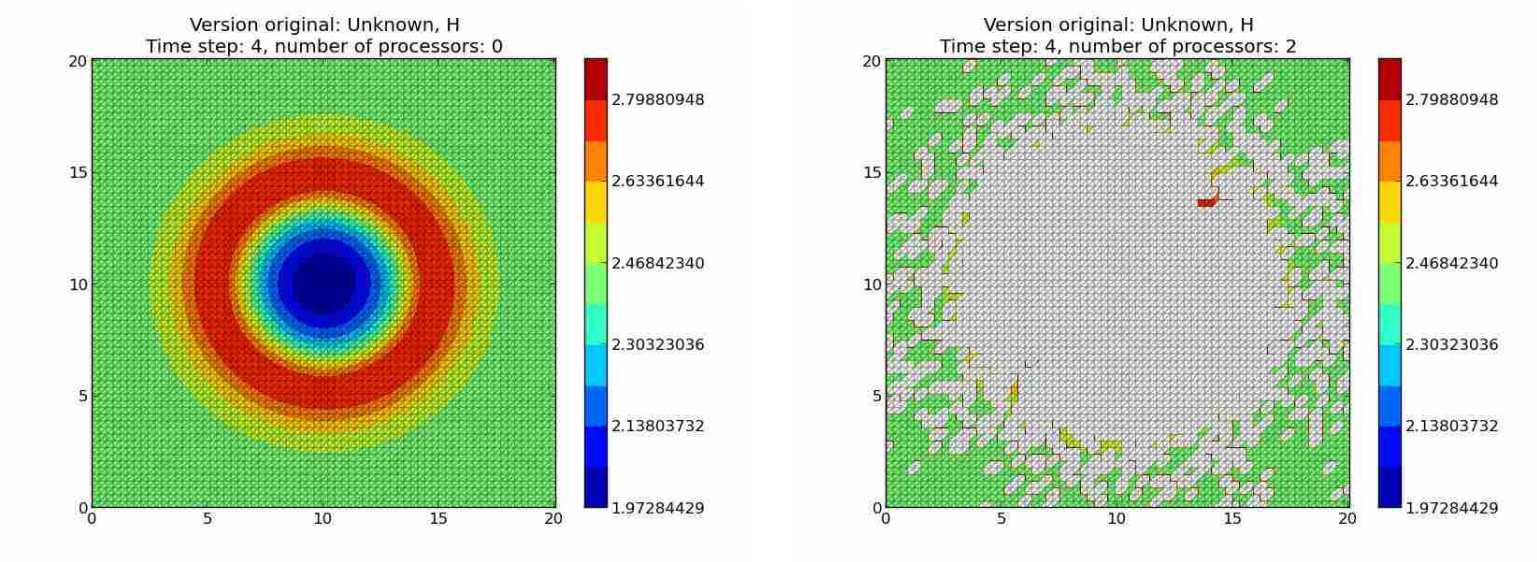
time step = 4



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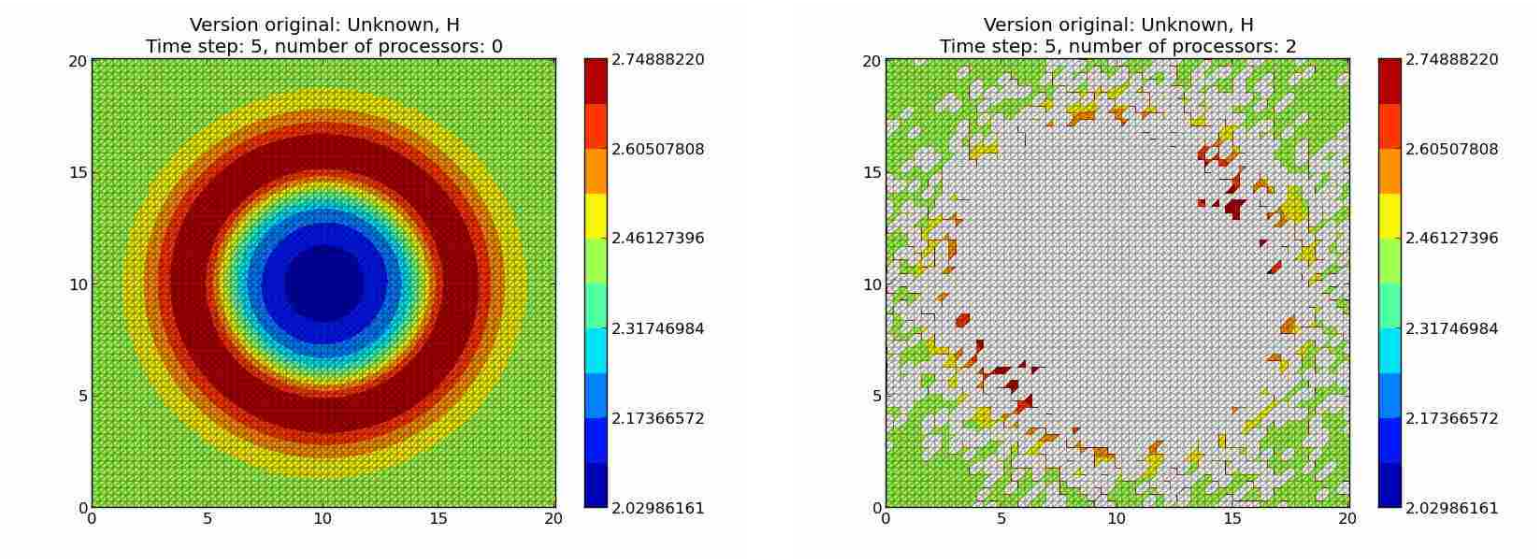
Numerical reproducibility?

time step = 5



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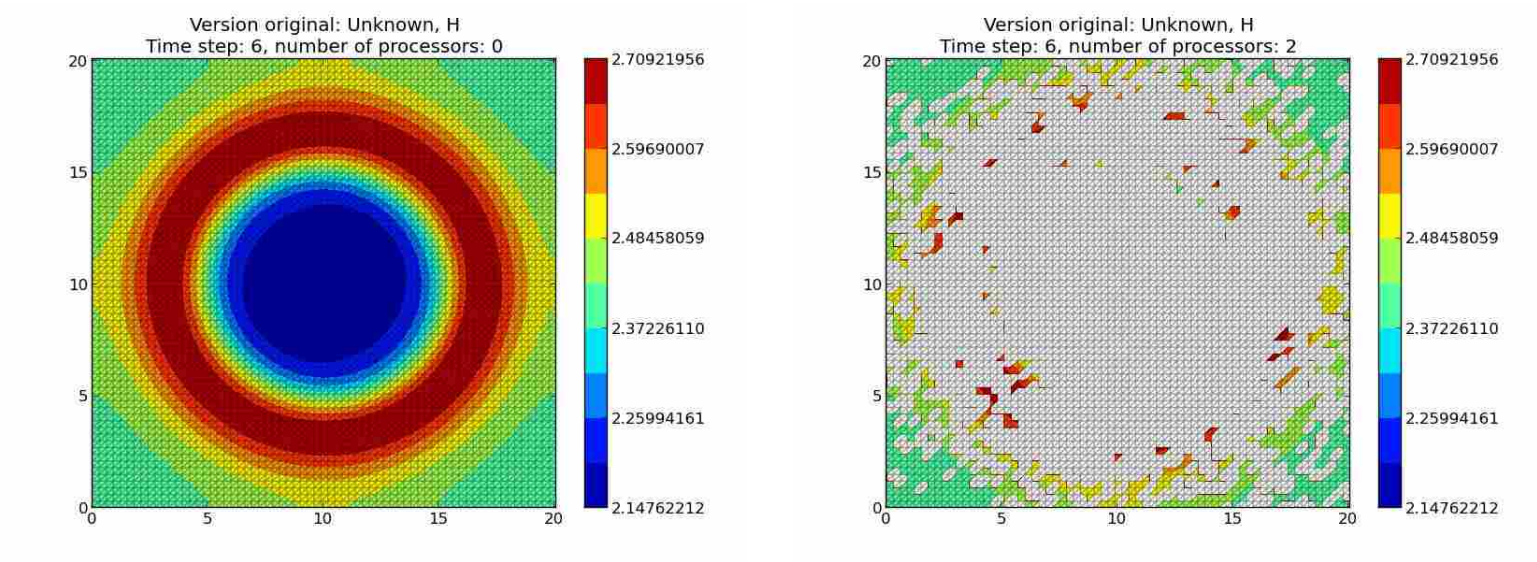
Numerical reproducibility?

time step = 6



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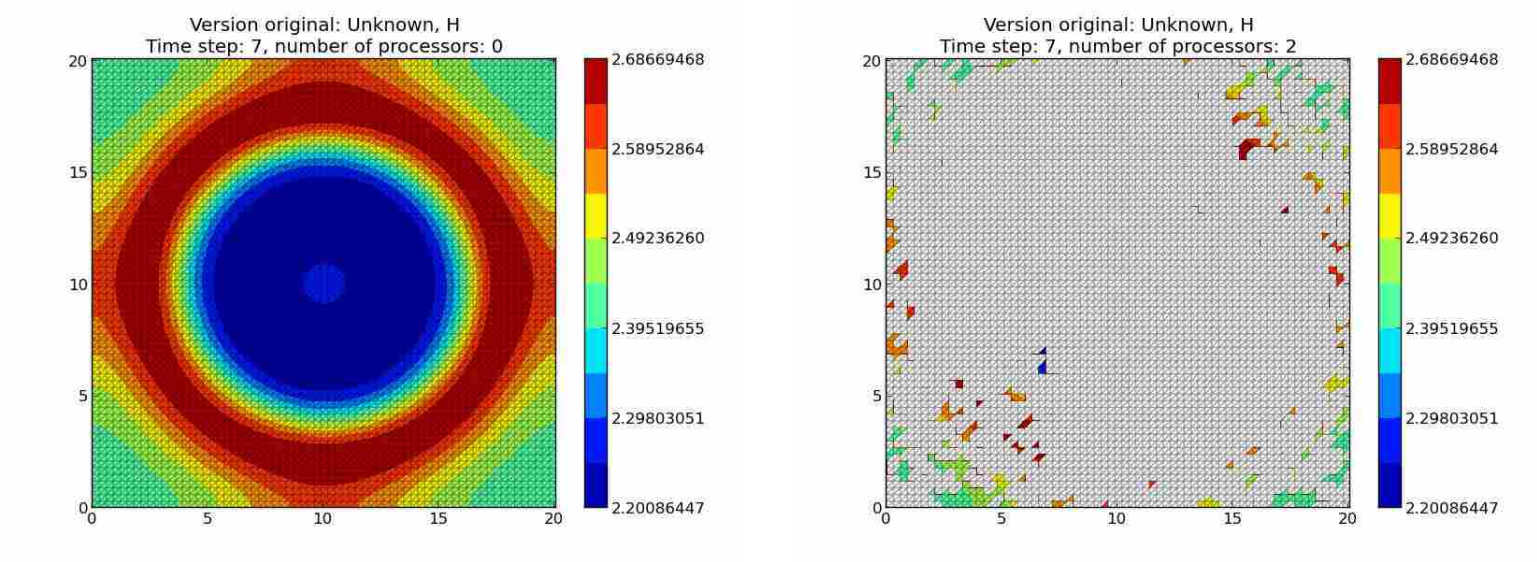
Numerical reproducibility?

time step = 7



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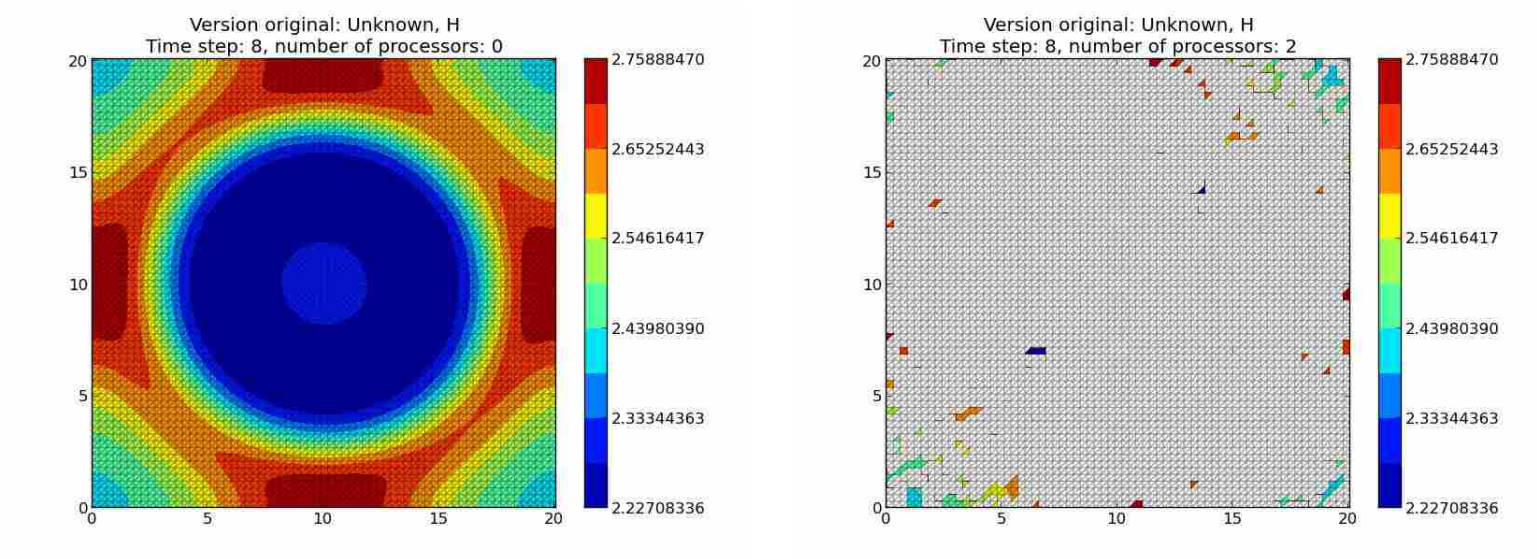
Numerical reproducibility?

time step = 8



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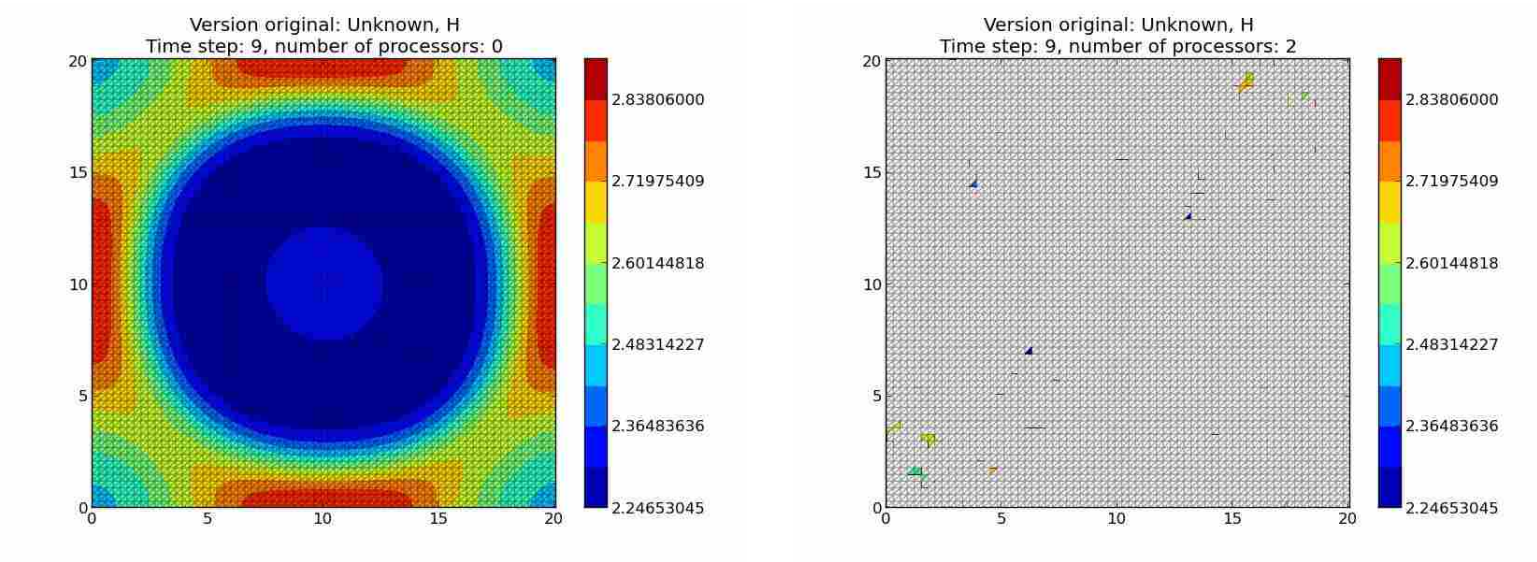
Numerical reproducibility?

time step = 9



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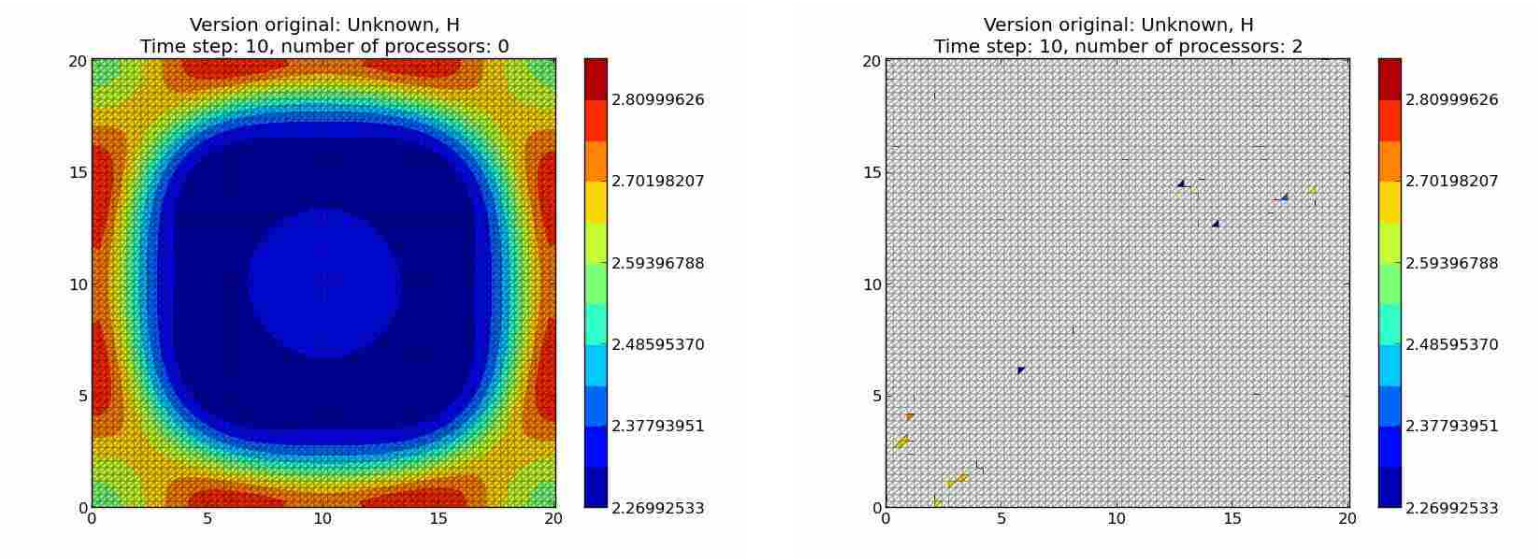
Numerical reproducibility?

time step = 10



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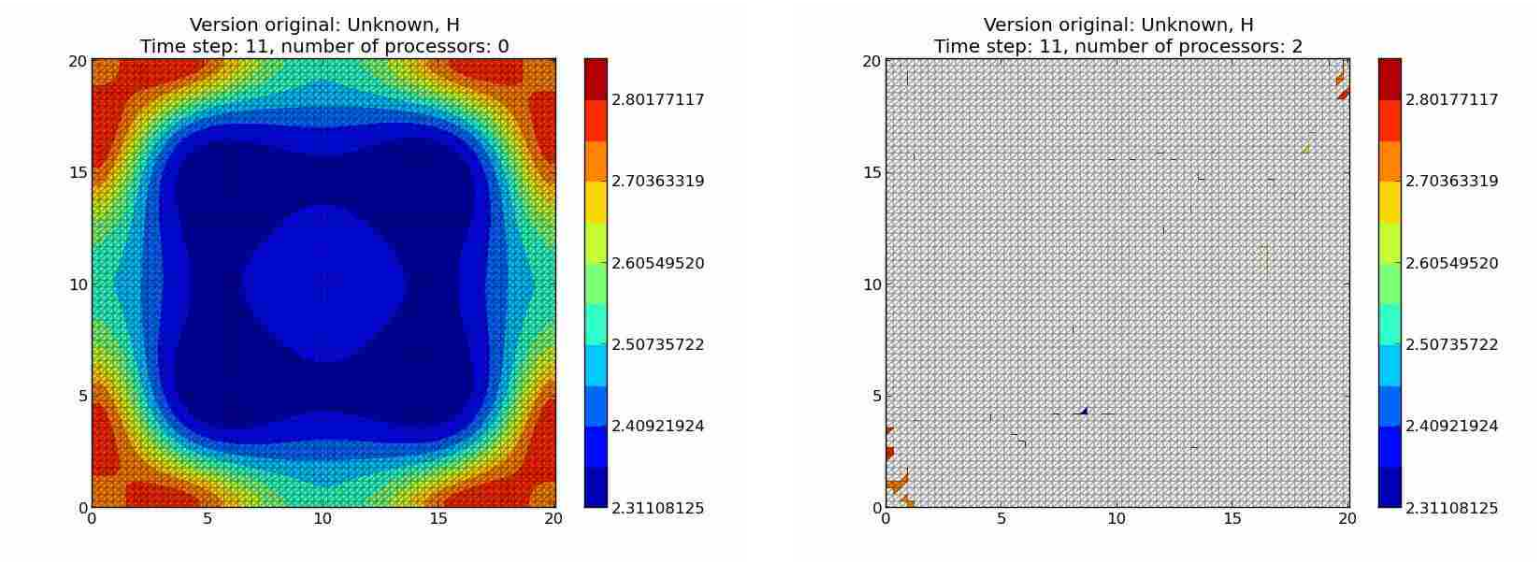
time step = 11



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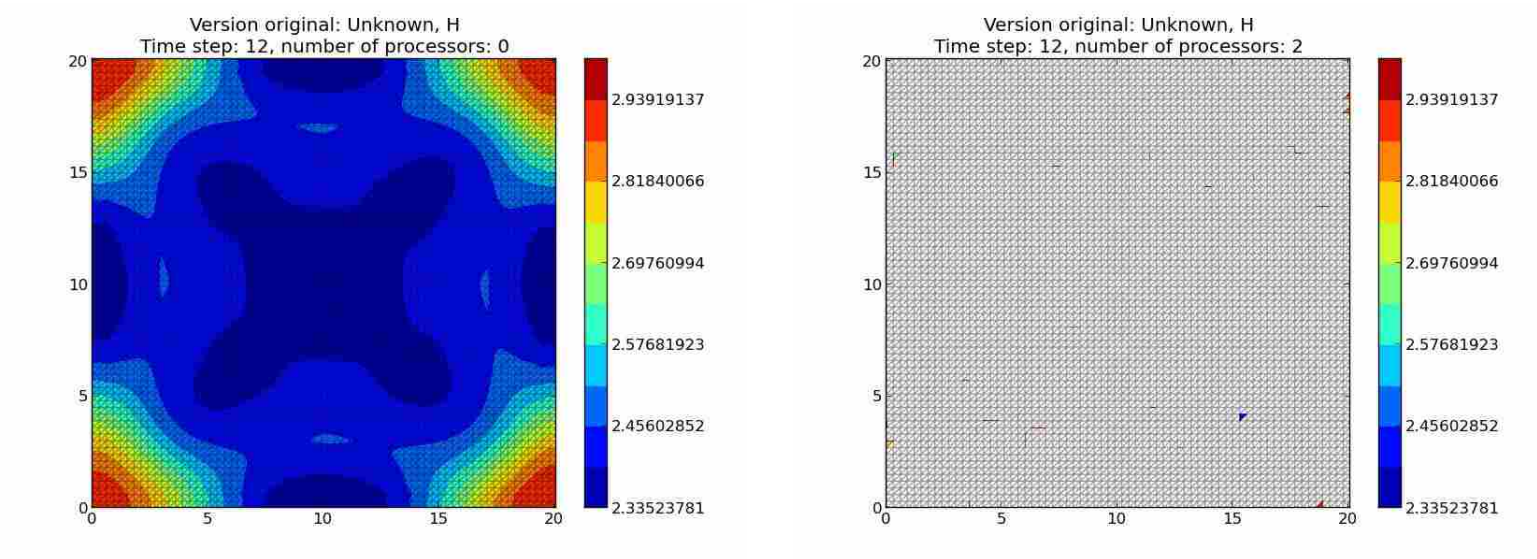
time step = 12



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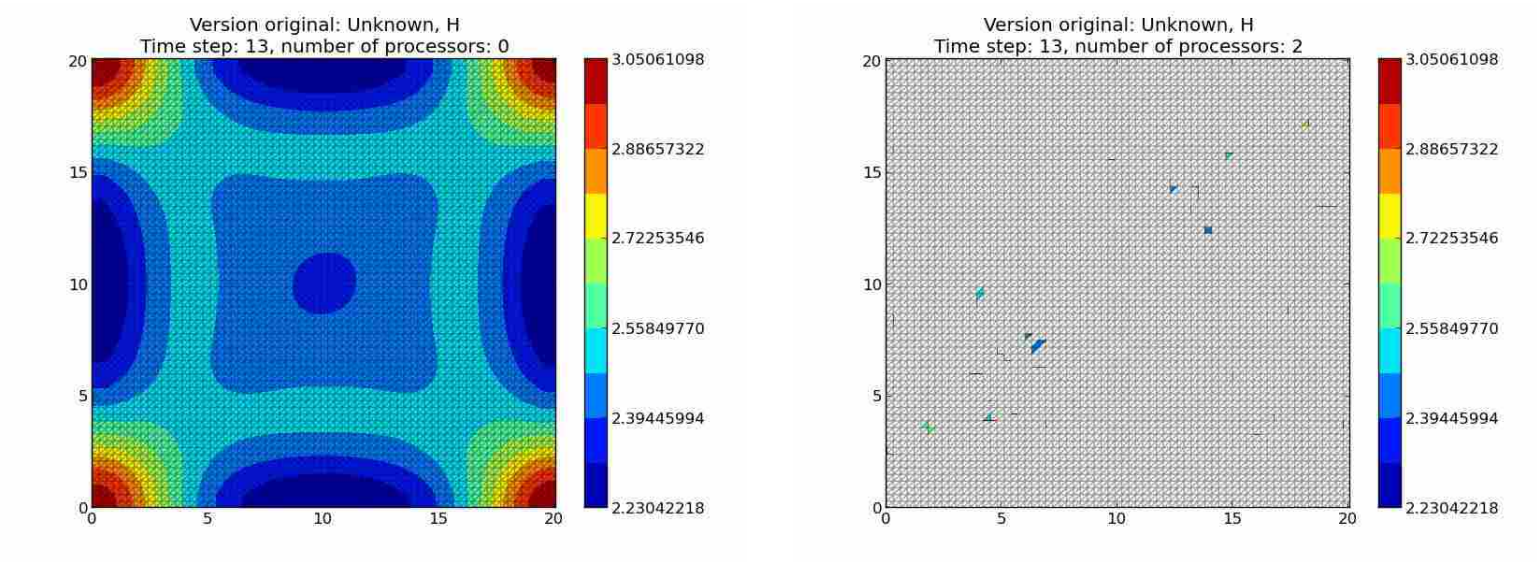
Numerical reproducibility?

time step = 13



Sequential

Parallel $p = 2$

Courtesy of P. Langlois and R. Nheili

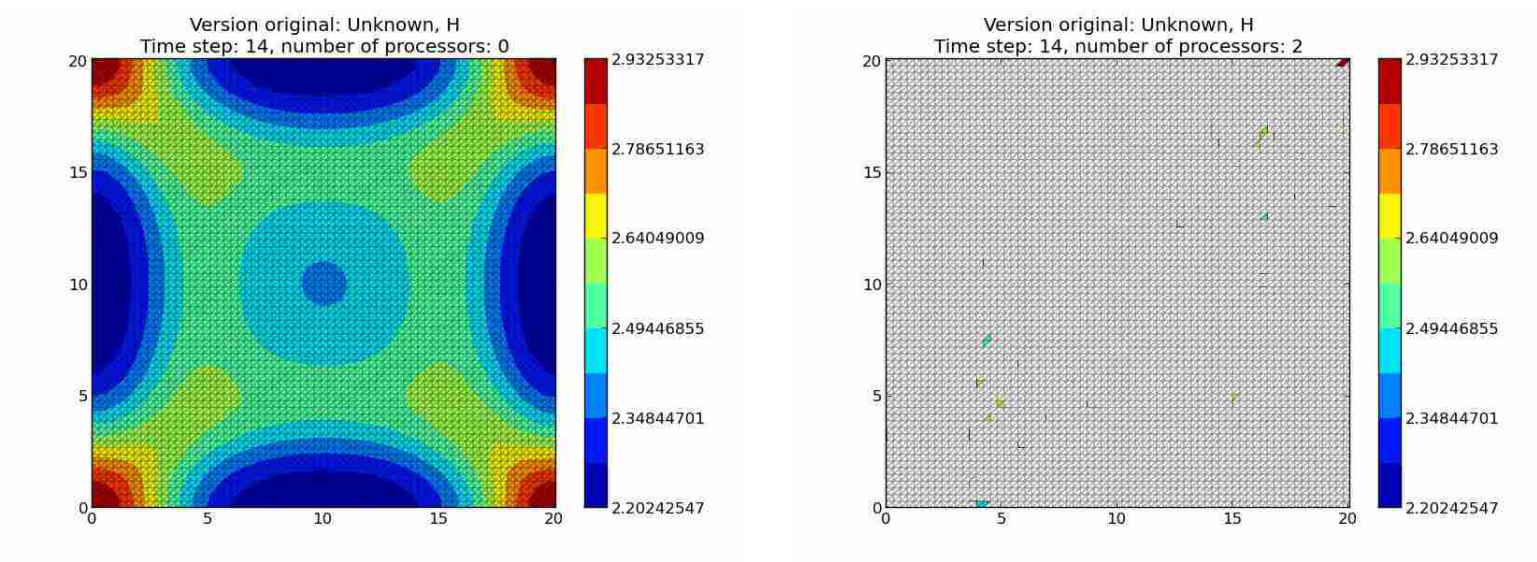
All I care about is the algorithm output

Did I mention we have parallel machines nowadays? 😉

A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 14



Sequential

Parallel $p = 2$

Courtesy of P. Langlois and R. Nheili

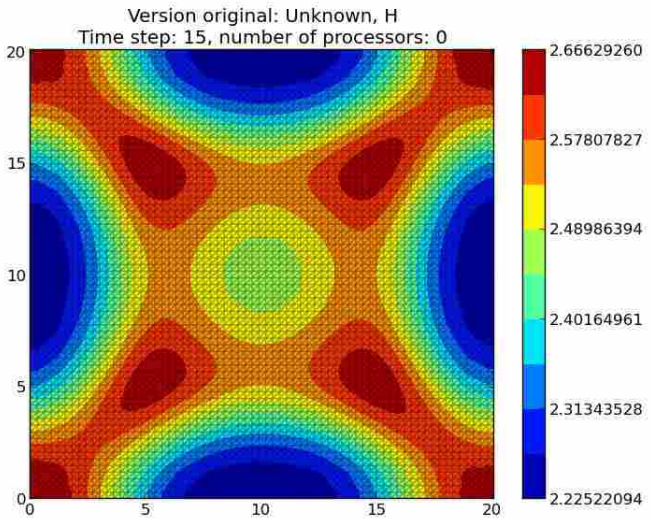
All I care about is the algorithm output

Did I mention we have parallel machines nowadays? 😉

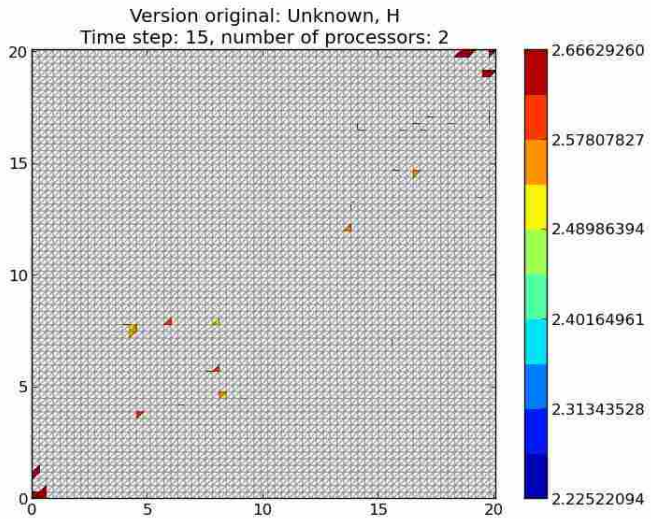
A white plot displays a non-reproducible value

NO numerical reproducibility!

time step = 15



Sequential



Parallel $p = 2$

Courtesy of P. Langlois and R. Nheili

All I care about is the algorithm output

Did I mention we have parallel machines nowadays? 😉

These numerical issues can become quite harmful in real use cases.

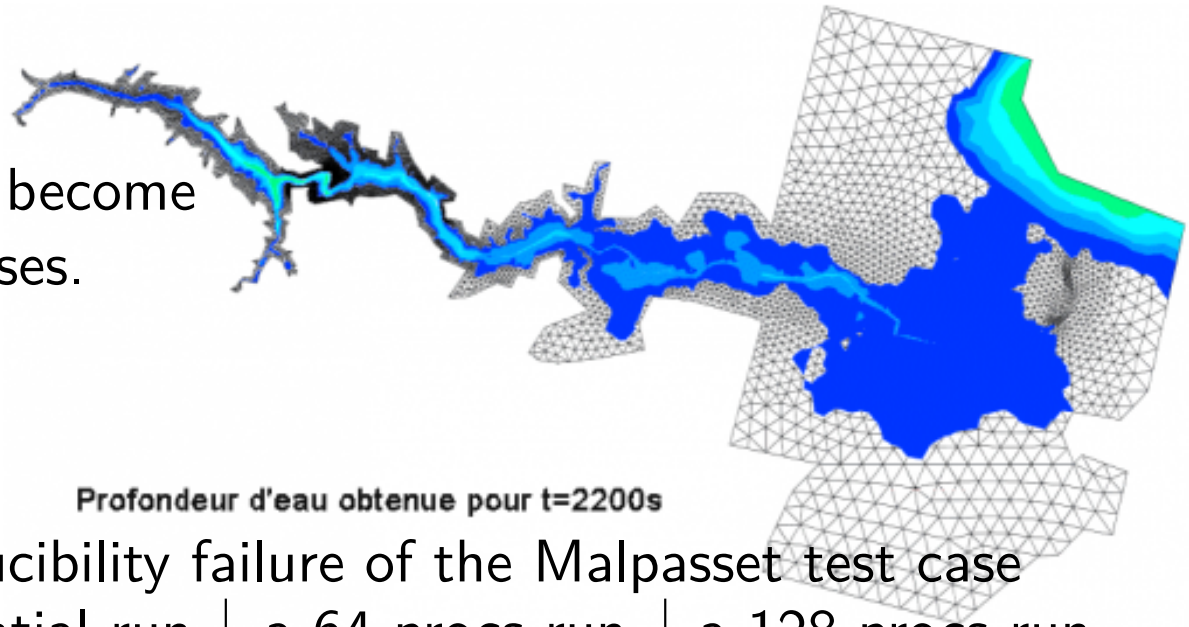


TABLE 1.1: Reproducibility failure of the Malpasset test case

	The sequential run	a 64 procs run	a 128 procs run
depth H	0.3500122E-01	0.2748817E-01	0.1327634E-01
velocity U	0.4029747E-02	0.4935279E-02	0.4512116E-02
velocity V	0.7570773E-02	0.3422730E-02	0.7545233E-02

Numerical reproducibility?: Approximations in the model, in in the algorithm, in its implementation, in its execution.

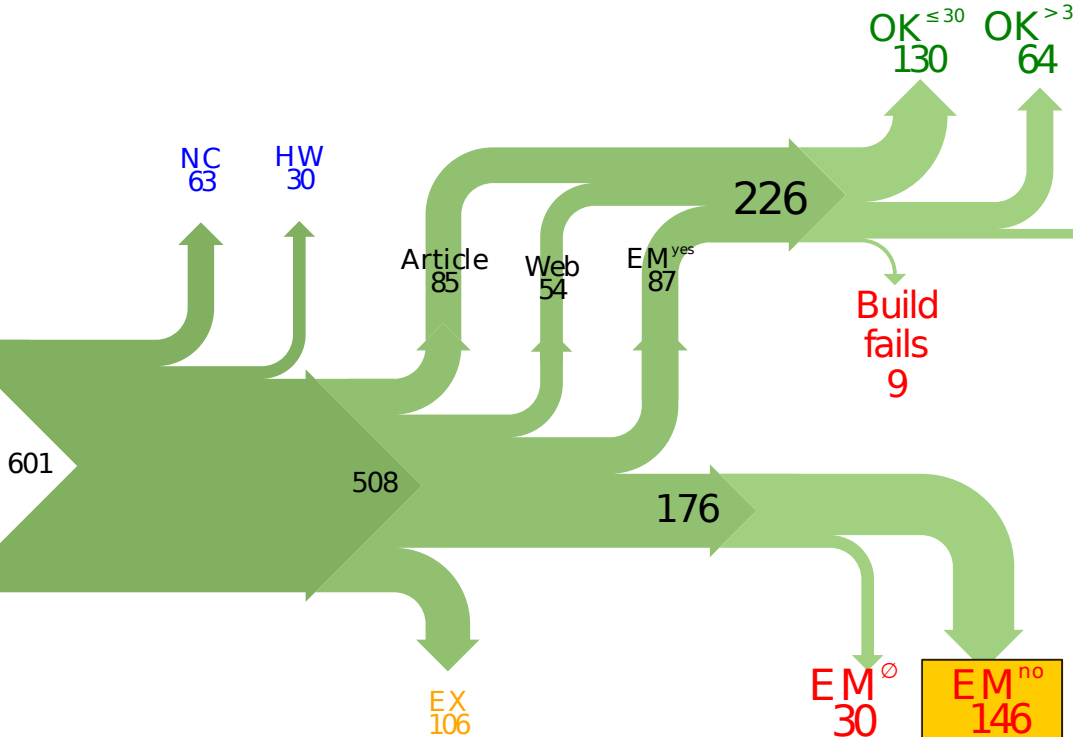
The whole chain needs to be revisited.

Courtesy of P. Langlois and R. Nheili

Outline

Lack of reproducibility is foremost a cultural matter

Collberg, Christian *et Al.*, *Measuring Reproducibility in Computer Systems Research*, http://reproducibility.cs.arizona.edu/



- 8 ACM conferences (ASPLOS'12, CCS'12, OOPSLA'12, OSDI'12, PLDI'12, SIGMOD'12, SOSP'11, VLDB'12) and 5 journals
- EM^{no} = the code cannot be provided

The Dog Ate my Homework !!!

- Versioning Problems

Thanks for your interest in the implementation of our paper. The good news is that I was able to find some code. I am just hoping that it is a stable working version of the code, and matches the implementation we finally used for the paper. Unfortunately, I have lost some data when my laptop was stolen last year. The bad news is that the code is not commented and/or clean.

Attached is the ⟨system⟩ source code of our algorithm. I'm not very sure whether it is the final version of the code used in our paper, but it should be at least 99% close. Hope it will help.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices

Unfortunately, the server in which my implementation was stored had a disk crash in April and three disks crashed simultaneously. While the help desk made significant effort to save the data, my entire implementation for this paper was not found.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon

Unfortunately the current system is not mature enough at the moment, so it's not yet publicly available. We are actively working on a number of extensions and things are somewhat volatile. However, once things stabilize we plan to release it to outside users. At that point, we would be happy to send you a copy.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release

I am afraid that the source code was never released. The code was never intended to be released so is not in any shape for general use.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left

⟨STUDENT⟩ was a graduate student in our program but he left a while back so I am responding instead. For the paper we used a prototype that included many moving pieces that only ⟨STUDENT⟩ knew how to operate and we did not have the time to integrate them in a ready-to-share implementation before he left. Still, I hope you can build on the ideas/technique of the paper.

Unfortunately, the author who has done most of the coding for this paper has passed away and the code is no longer maintained.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code

Since this work has been done at ⟨COMPANY⟩ we don't open-source code unless there is a compelling business reason to do so. So unfortunately I don't think we'll be able to share it with you.

The code owned by ⟨COMPANY⟩, and AFAIK the code is not open-source. Your best bet is to reimplement :(Sorry.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code
- Proprietary Academic Code

Unfortunately, the ⟨SYSTEM⟩ sources are not meant to be opensource (the code is partially property of ⟨UNIVERSITY 1⟩, ⟨UNIVERSITY 2⟩ and ⟨UNIVERSITY 3⟩.)

If this will change I will let you know, albeit I do not think there is an intention to make the ⟨SYSTEM⟩ sources opensource in the near future.

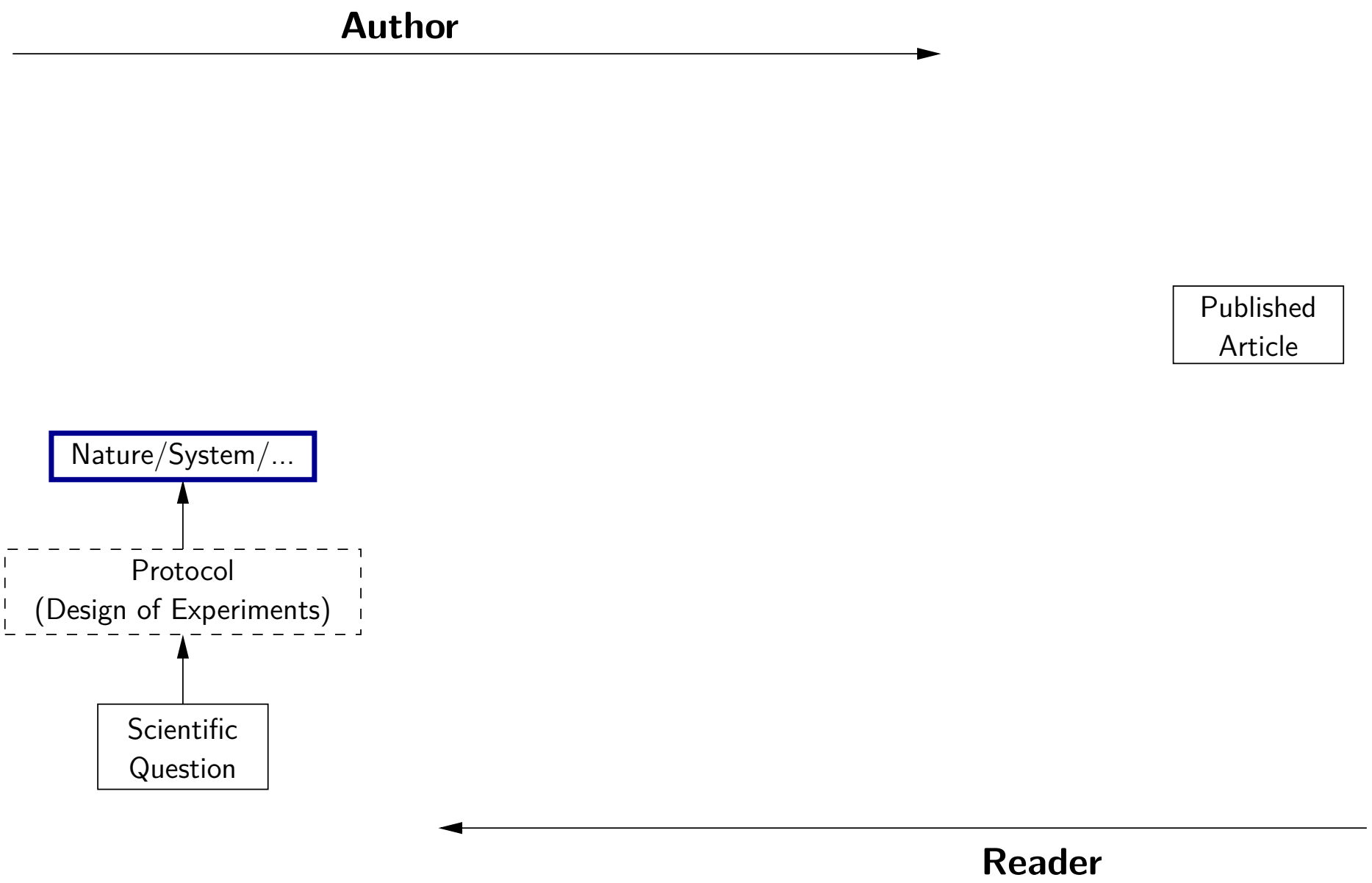
If you're interested in obtaining the code, we only ask for a description of the research project that the code will be used in (which may lead to some joint research), and we also have a software license agreement that the University would need to sign.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code
- Proprietary Academic Code
- Research vs. Sharing
- ...
- ...

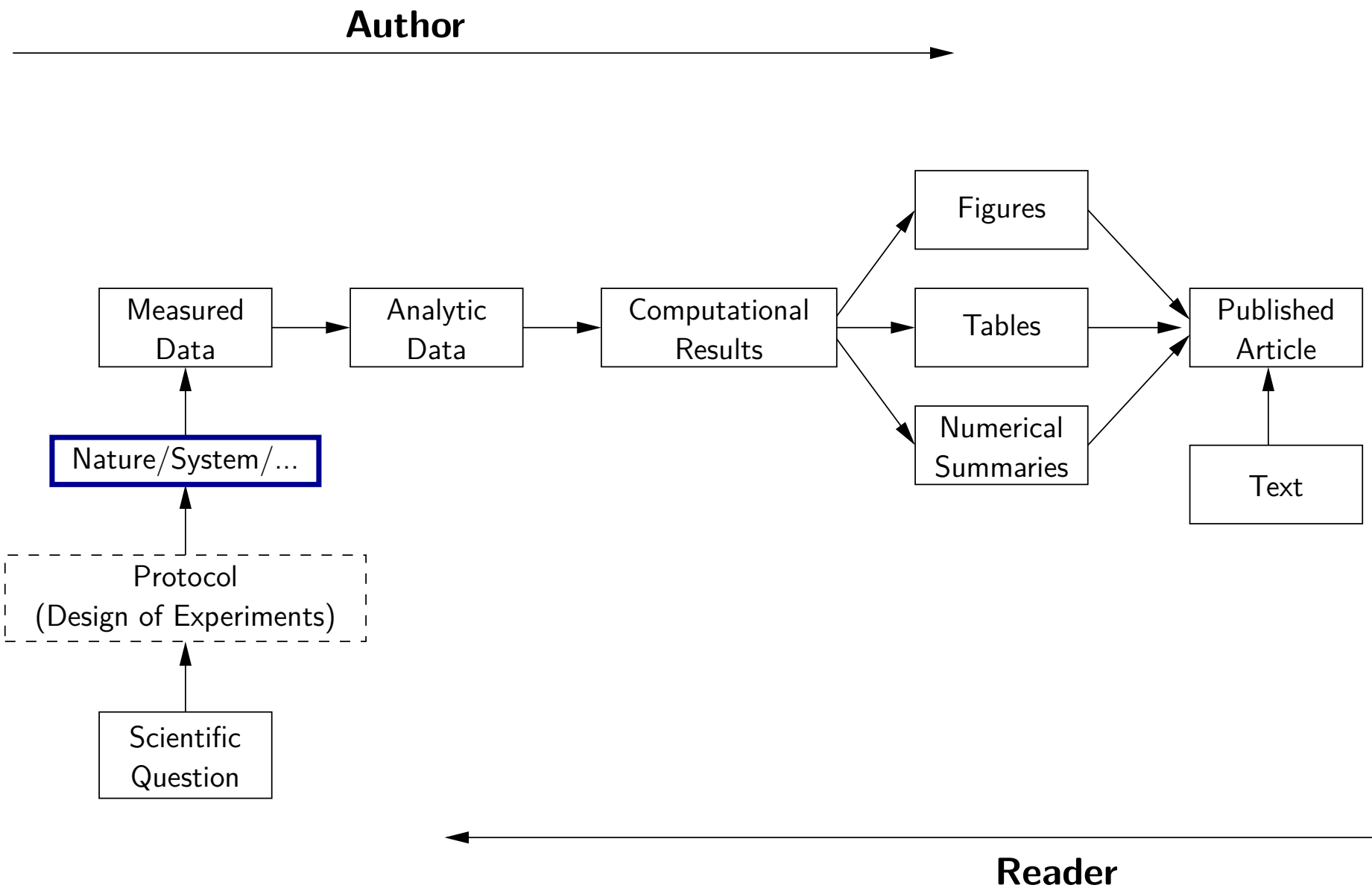
In the past when we attempted to share it, we found ourselves spending more time getting outsiders up to speed than on our own research. So I finally had to establish the policy that we will not provide the source code outside the group.

Reproducible Research: Trying to Bridge the Gap



Inspired by Roger D. Peng's lecture on reproducible research, May 2014

Reproducible Research: Trying to Bridge the Gap



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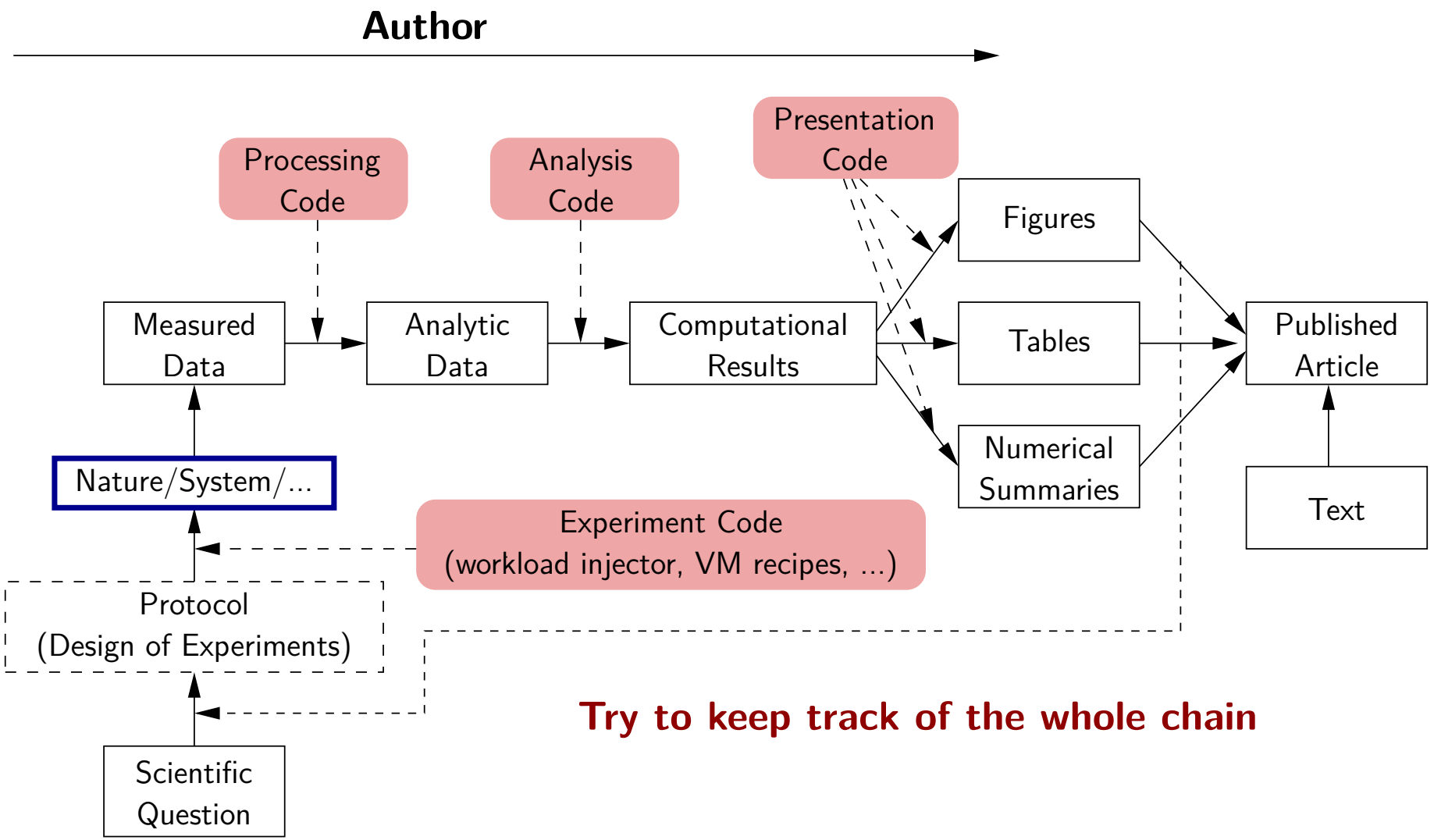

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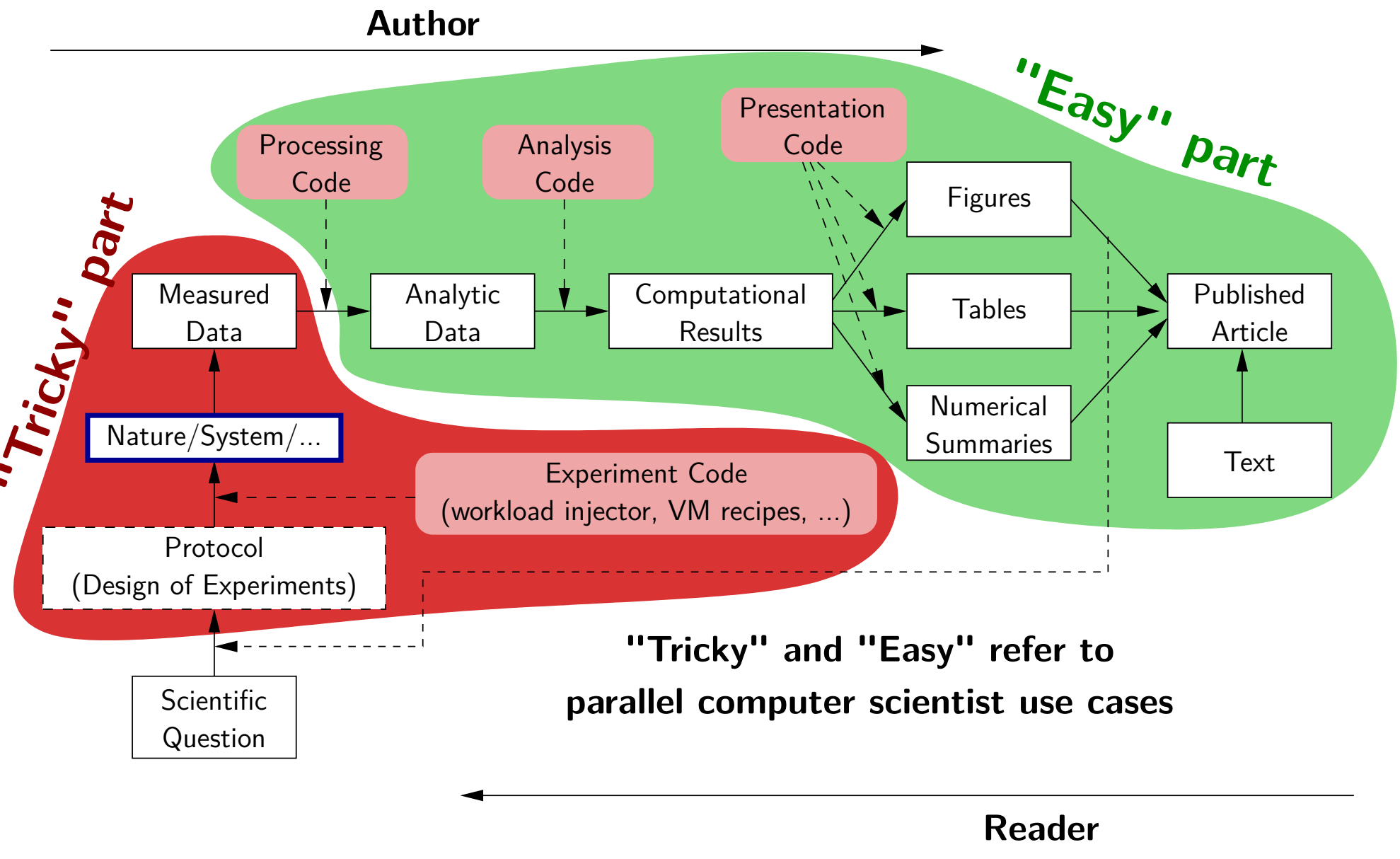


Inspired by Roger D. Peng's lecture on reproducible research, May 2014

Paradigm Shift

1. Lack of information, data access
   $\rightsquigarrow$ *The right tracking/sharing tools*
2. Lack of technical and scientific rigor
   $\rightsquigarrow$ *Better methodology (e.g., training in stats)*
3. Computation/programming mistakes
   $\rightsquigarrow$ *Continuous integration, code review, environment control, numerical analysis, . . .*
4. Little incentive to care/share/. . .
   $\rightsquigarrow$ *The contribution evaluation processs (publication, recruiting, . . .) needs to evolve*

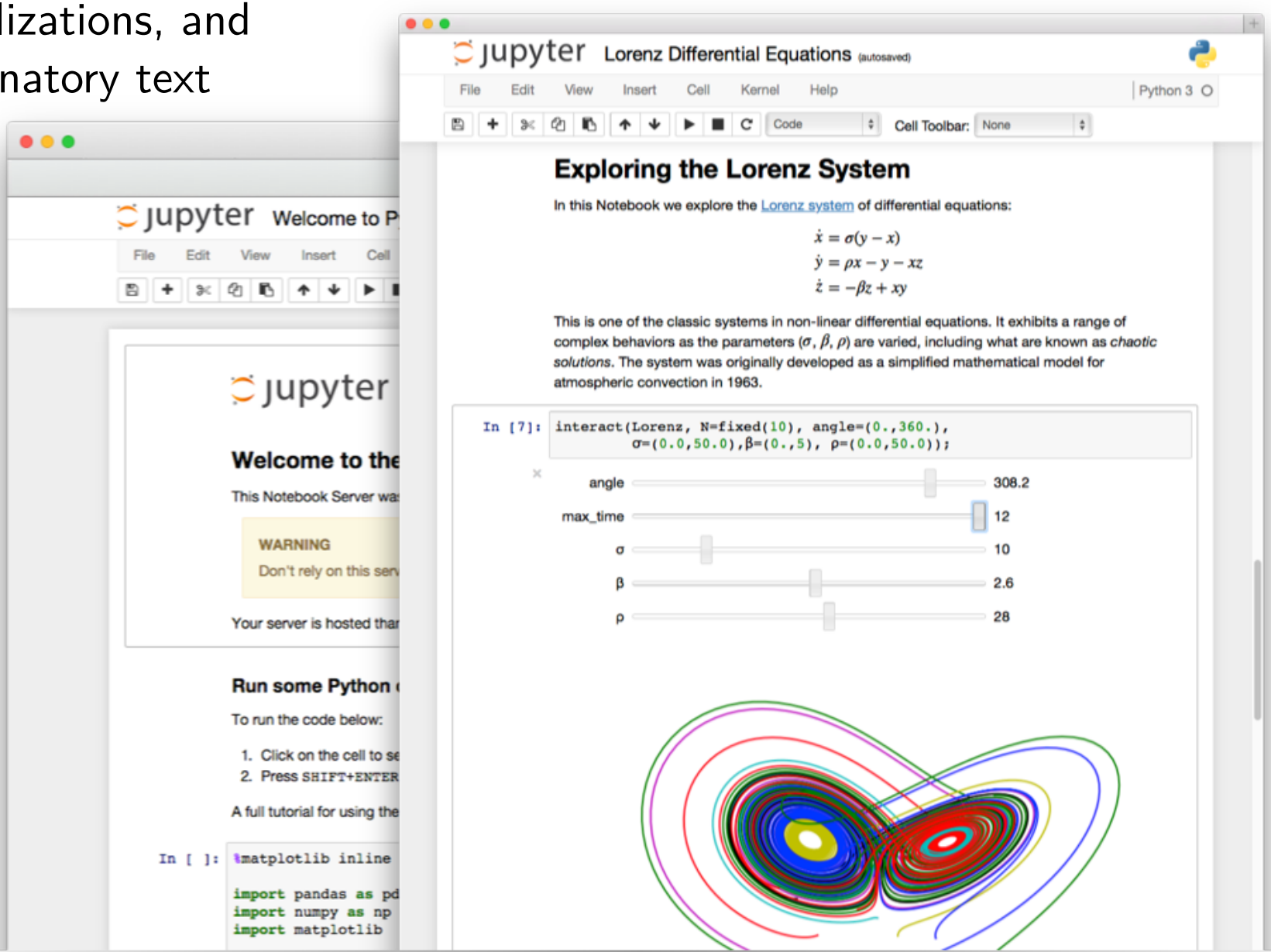
Transparency increases the chances of finding mistakes
and getting rid of them

Outline

Outline

Ipython/Jupyter Notebook

Web app: create and share documents that contain live code, equations, visualizations, and explanatory text



Computational Document (Jupyter Notebook)

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)
```

```
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```
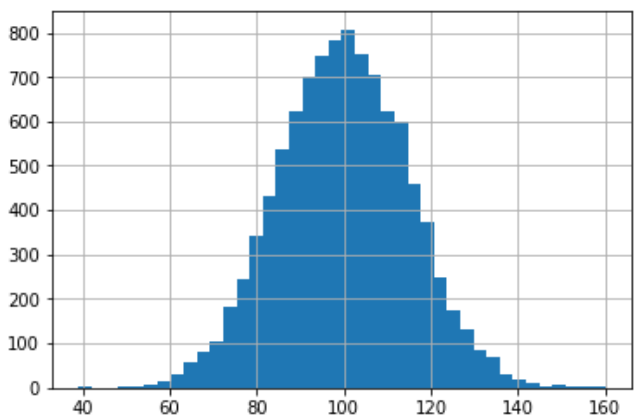

On peut inclure des formules mathématiques comme $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ et des *dessins qui n'ont rien à voir* avec π (si ce n'est une constante de normalisation... ☺).



Computational Document (Jupyter Notebook)

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
```

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```
Mon ordinateur m'indique que $\pi$ vaut *approximativement*
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In [1]:

Hide Prompts Hide Code Hide Outputs

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from math import *
print(pi)
```

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Hide Prompts Hide Code Hide Outputs

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Hide Prompts Hide Code Hide Outputs

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Out[2]:

```
3.1437198694098765
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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()
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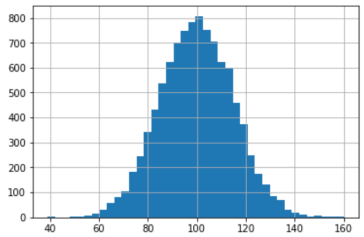

Document final

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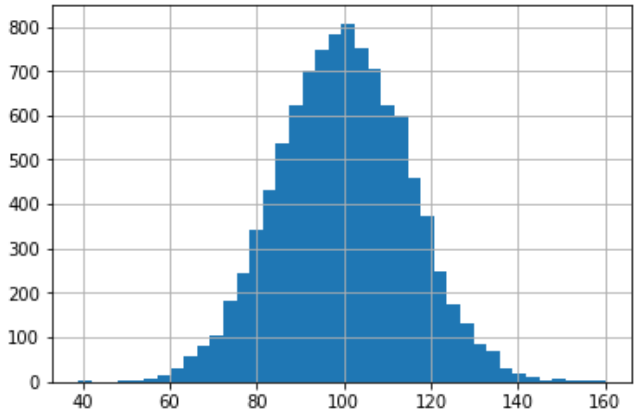

Computational Document (Jupyter Notebook)

Document initial dans son environnement

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Code CellToolbar

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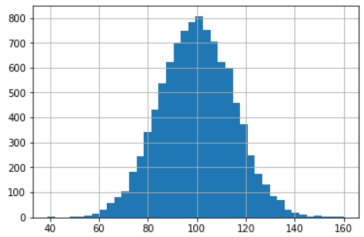

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Document final

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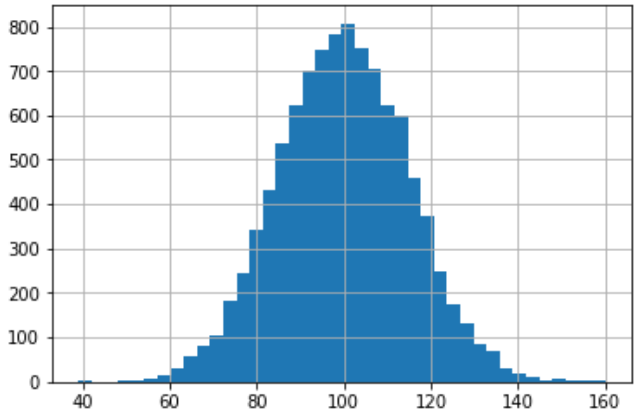

Computational Document (Jupyter Notebook)

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Code CellToolbar

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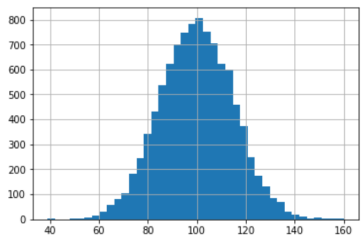

Code

Document final

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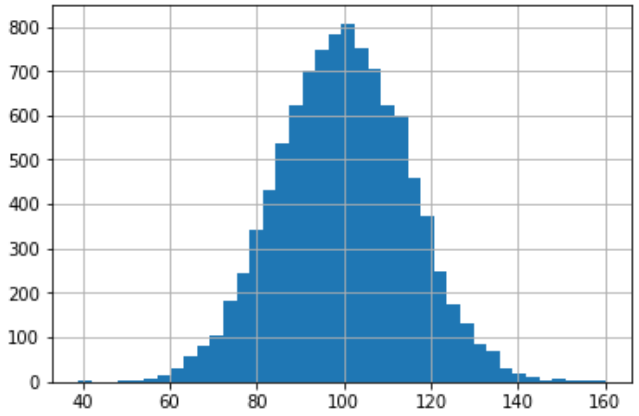

Computational Document (Jupyter Notebook)

Document initial dans son environnement

jupyter example_pi (autosaved)

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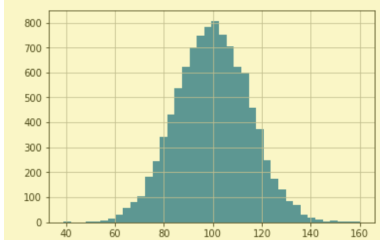

Résultats

Document final

Un document computationnel

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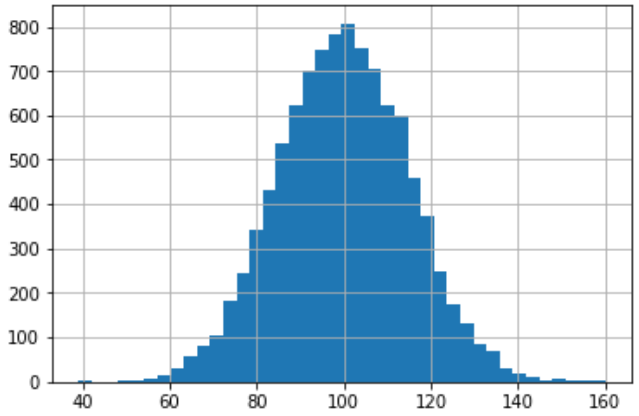

Computational Document (Jupyter Notebook)

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

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# Un document computationnel
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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
__approximation__ :
```

In [2]:

Hide Prompts Hide Code Hide Outputs

```
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
```

Hide Prompts Hide Code Hide Outputs

```
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... ☺).
```

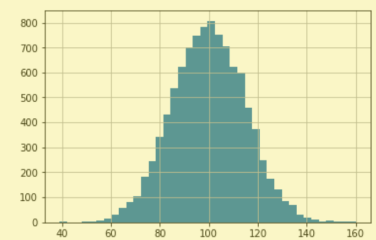
In [3]:

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

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
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```
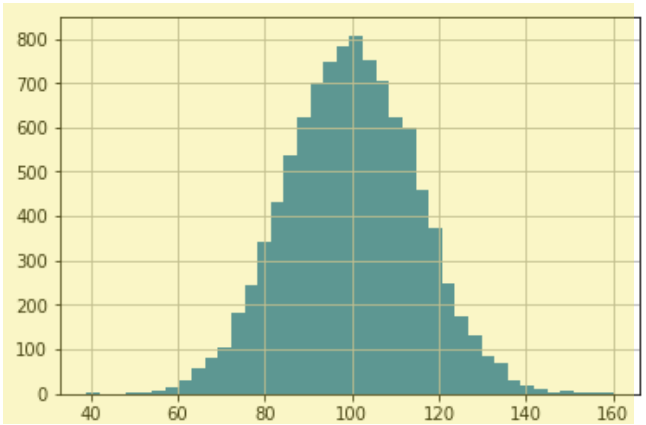
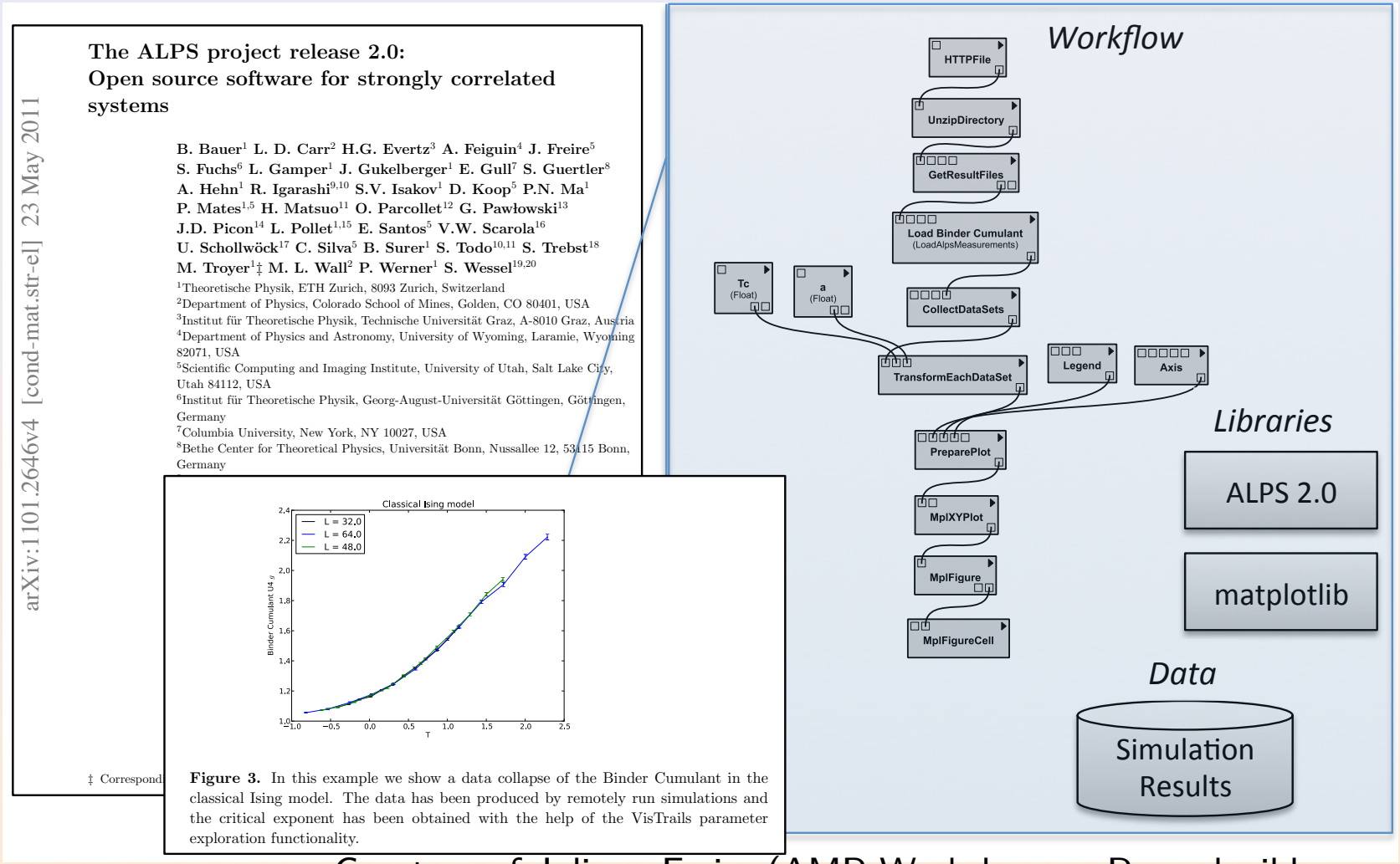

```
3.1437198694098765
```

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... ☺).



Vistrails: a Workflow Engine for Provenance Tracking

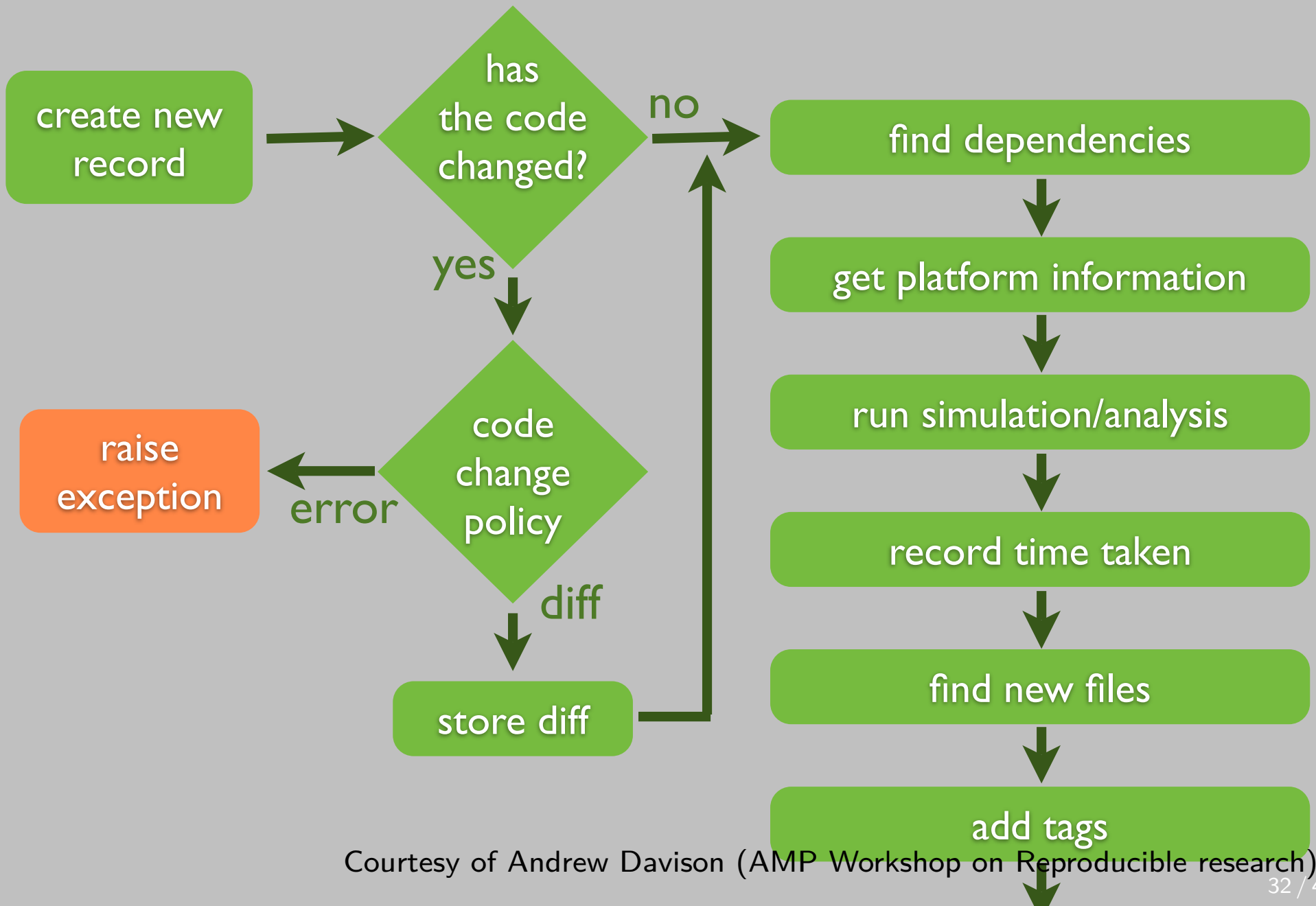
An *Provenance-Rich* Paper: ALPS2.0



Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

[Reproducible ISTAT 2011]

Sumatra: an "experiment engine" that helps taking notes



Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: an "experiment engine" that helps taking notes

```
$ smt comment 20110713-174949 "Eureka! Nobel prize
here we come."
```

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: an "experiment engine" that helps taking notes

```
$ smt tag “Figure 6”
```

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: an "experiment engine" that helps taking notes

Sumatra: TestProject: List of records

http://127.0.0.1:8002/

Google

TestProject: List of records

Delete / include data	Label	Reason	Outcome	Duration	Processes	Simulator		Script			Date	Time	Tags
						Name	Version	Repository	Main file	Version			
☐	20100709-154255		'Eureka! Nobel prize here we come.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:42:55	
☐	20100709-154309			0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:09	
☐	haggling	'determine whether the gourd is worth 3 or 4 shekels'	'apparently, it is worth NaN shekels.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:20	fooba
☐	20100709-154338	'test effect of a smaller time constant'		0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:38	
☐	haggling_repeat	Repeat experiment haggling	The new record exactly matches the original.	0.58 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:47	

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

My daily solution: Emacs/Org-mode

My journal a single file

- Chronological organization with TAGS
- Heterogenous information
- Code execution is convenient

My students' laboratory notebooks

- Conventions
- $\approx$ Chronological organization
- Track info about experiments (who, what, when, how, why) and data analysis

Replicable articles

- Easily built on the previous documents
- Many hidden sections (data download, perl/R scripts)
- Sources connect figures with data and meta-data

Outline

Complex Environments

```
1 import matplotlib
2 print(matplotlib.__version__)
```

```
1 2.1.1
```

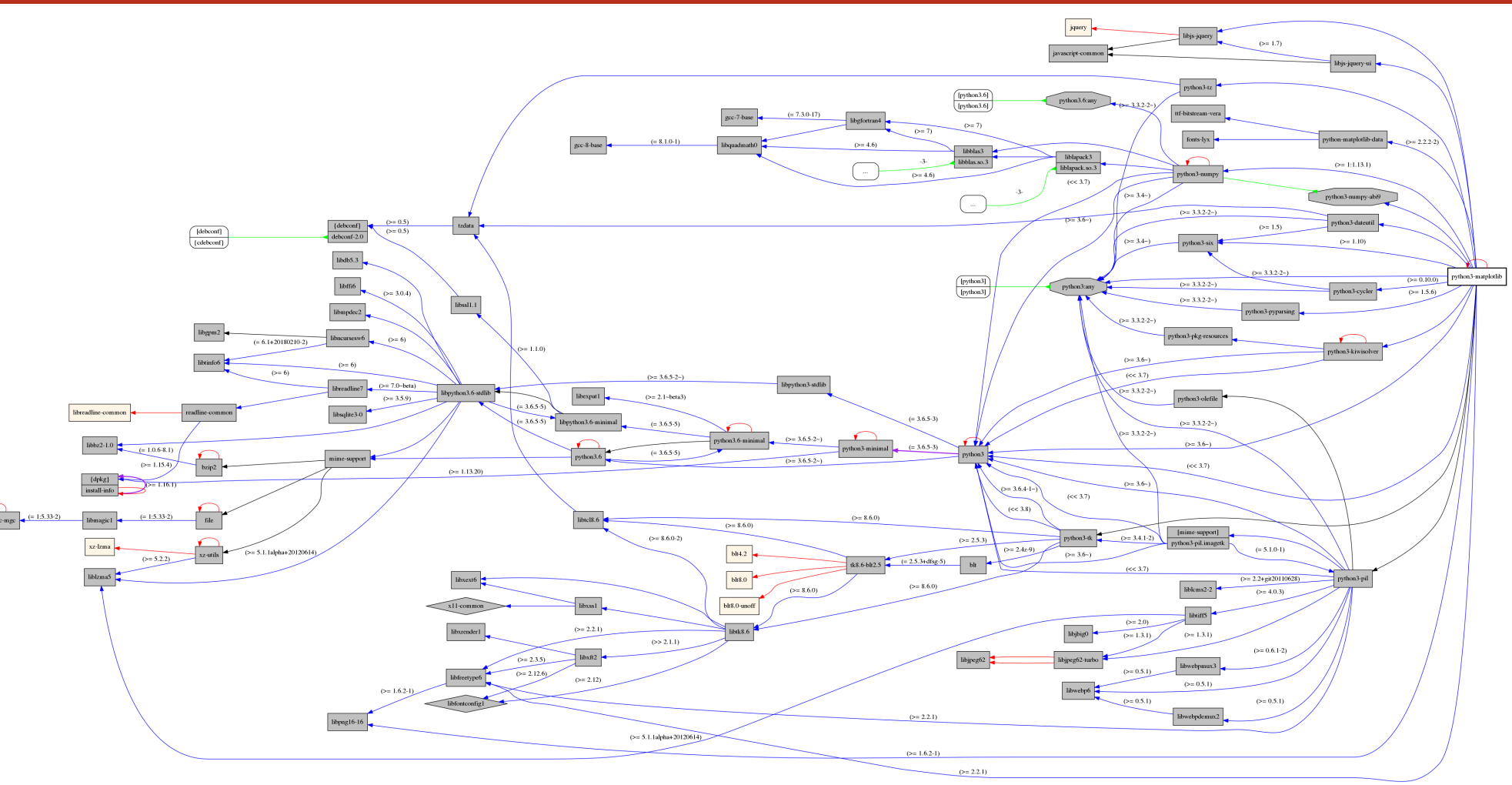
Complex Environments

```
1 import matplotlib
2 print(matplotlib.__version__)
```

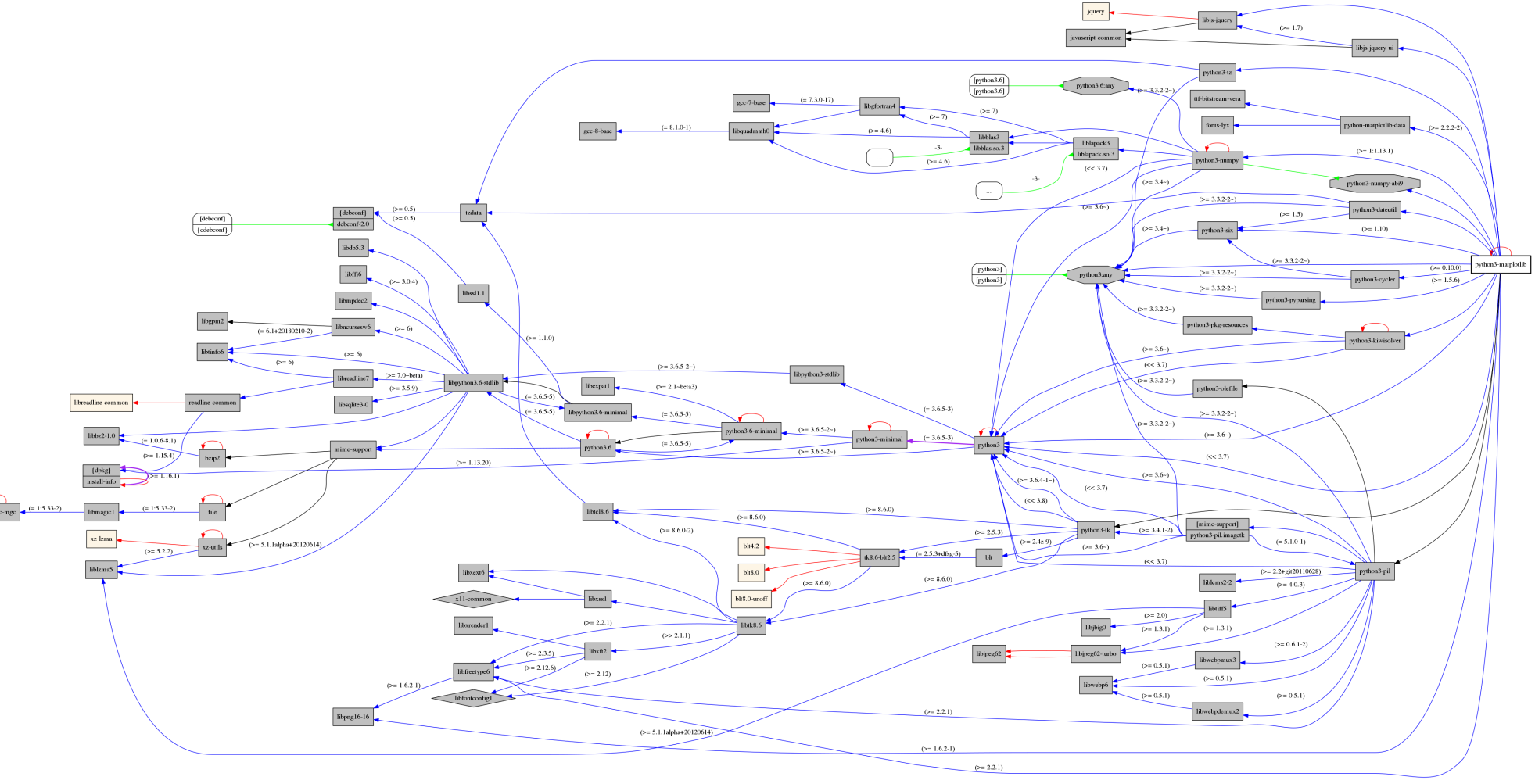
```
1 2.1.1
```

```
1 Version: 2.1.1-2
2 Depends: python3-dateutil, python-matplotlib-data (>= 2.1.1-2),
3 python3-pyparsing (>= 1.5.6), python3-six (>= 1.10), python3-tz,
4 libjs-jquery, libjs-jquery-ui, python3-numpy (>= 1:1.13.1),
5 python3-numpy-abi9, python3 (<< 3.7), python3 (>= 3.6~),
6 python3-cycler (>= 0.10.0), python3:any (>= 3.3.2-2~), libc6 (>=
7 2.14), libfreetype6 (>= 2.2.1), libgcc1 (>= 1:3.0), libpng16-16
8 (>= 1.6.2-1), libstdc++6 (>= 5.2), zlib1g (>= 1:1.1.4)
```

Complex Environments



Complex Environments



Virtual images or *Docker containers* allow to freeze environements

Two approaches: *preserve the mess* vs. *encourage cleanliness*

Reprozip

Automagically pack your experiment to fight dependency hell

ON THE ORIGINAL MACHINE

```
$ pip install reprozip
$ reprozip trace ./myexperiment -my --options inputs/somefile.csv other_file_here.bin
experiment: 0%... 25%... 50%... 75%... 100%
result: 42.137
Configuration file written in .reprozip/config.yml
Edit that file then run the packer -- use 'reprozip pack -h' for help
$ reprozip pack my_experiment.rpz
[REPROZIP] 17:26:42.588 INFO: Creating pack my_experiment.rpz...
[REPROZIP] 17:26:42.589 INFO: Adding files from package coreutils...
[REPROZIP] 17:26:42.601 INFO: Adding files from package libc6...
[REPROZIP] 17:26:42.906 INFO: Adding other files...
[REPROZIP] 17:26:43.450 INFO: Adding metadata...
```

ON ANOTHER MACHINE

```
$ pip install reprounzip[all]
$ reprounzip vagrant setup my_experiment.rpz mydirectory
Bringing machine 'default' up with 'virtualbox' provider...
==> default: Importing base box 'remram/debian-7-amd64'...
==> default: Booting VM...
==> default: Machine booted and ready!
==> default: Running provisioner: shell...
$ reprounzip vagrant run mydirectory
experiment: 0%... 25%... 50%... 75%... 100%
result: 42.137
$ reprounzip vagrant upload /tmp/new_config:global-config
$ reprounzip vagrant run mydirectory --cmdline ./myexperiment --other --options
inputs/somefile.csv
experiment: 0%... 25%... 50%... 75%... 100%
result: -17.814
```

Other options:

~~CARE~~, CDE, Reprozip, Pipenv | Docker, Singularity | Spack, GUIX, NIX

Controlling experiments

- Naive way: sh + ssh + ...
- Better way: use a workflow management system (taverna, galaxy, kepler, vistrails, ...)
- Parallel/distributed experiments require specific experiment engines
  - Expo (2007-, G5K)
  - XPflow (2012-, G5K)
  - Execo (2013-, G5K)

  } although nothing specific to G5K

  - Plush (2006-, Planetlab)
  - OMF (2009-, Wireless)
  - Splay (2008), ...

  They differ in the underlying paradigms and the platforms for which they have been designed

  A survey of general-purpose experiment management tools for distributed systems, T. Buchert, C. Ruiz, L. Nussbaum, O. Richard, FGCS, 2014

- Control your **numerical results** (random generators, libraries, rounding and non-determinism, ...)

Outline

Hosting platforms

- Your webpage ☹
- Articles: Arxiv, HAL
- Code: Github or Institutional Gitlab
- Figshare, Zenodo ☺
- Companion websites (elsevier executable paper ☹, runmycode, exec&share, code ocean . . .)

This may seem easy but is quite tricky:

- Arbitrary limits can make your life painful
- Perennity (Roberto Di Cosmo's talks)
  - CodeSpaces murdered on Amazon, Google Code termination, Gitorious shutdown, . . .
  - Disruption of the web of reference: URLs decay (half-life of 4 years), DOIs have little guarantee, . . .

Outline

Publishing initiatives

Artifact evaluation and ACM badges Article appendix (SC)

Platforms Elsevier executable paper, ACM pushes for code ocean

Double blind vs. Open reviews plus "legal aspects"

RR-oriented & Open Journals IPOL

ReScience
Reproducible science is good. Replicated science is better.

Funding Agencies

US *NSF has released a new announcement encouraging submission of research projects relating to reproducibility and replicability.*
– Jim Kurose, Oct. 2016

The NIH is committed to promoting rigorous and transparent research in all areas of science supported by a variety of grant programs.
– NIH: Rigor and Reproducibility guidelines

Europe *In 2012, the European Commission encouraged all EU Member States to put public-funded research results in the public sphere in order to make science better and strengthen their knowledge-based economy.*
– Open Science (Open Access)

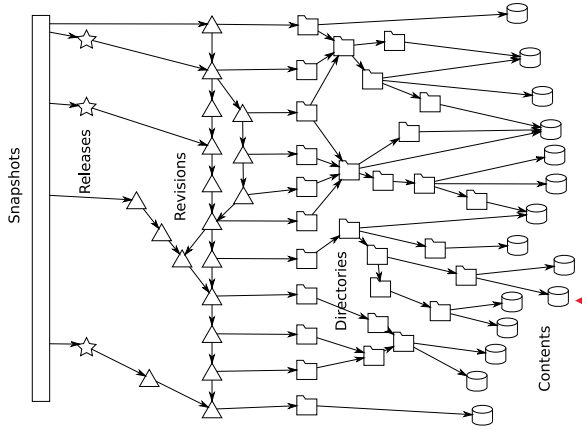
A key element will be capacity building to link literature and data in order to enable a more transparent evaluation of research and reproducibility of results. *– H2020-EINFRA-2014-2015*

Encouraging the re-use of research data generated by publically funded research projects *– Science with and for Society, 27 October 2017*

Outline

On the "technical" side (1/2)

- Better documenting what we do: Laboratory notebooks
  - Literate programming is great for analysis, and reproducible articles but does not go well yet with conducting experiments and workflows
  - A real adoption of such practice requires more storage and the ability to navigate in such information
- Better software engineering practice: Public releases, devops approach, reproducible builds, numerical aspects
  - Moving/evolving technology. Preservation ? Adoption ?
  - Should not slow down research
- Fighting against software/data degradation: Software Heritage, zenodo
  - Challenges: multiple! curation, access/privacy, exploitation, navigation, storage, ...

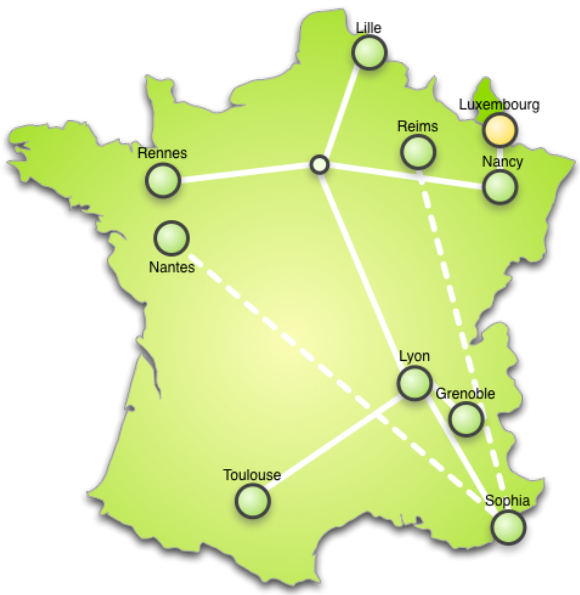


Software Heritage

THE GREAT LIBRARY OF SOURCE CODE

On the "technical" side (2/2)

- Better experimental practice and platforms: FIT IoT-lab, G5K are world leading experimental infrastructures; rely on standard simulators (SimGrid, NS3)
  - Maintenance cost, keeping in pace with technology, practices for prototype platforms, control, sharing of experimental conditions with others, experimental engines



- Need for convergence (SILEX) in term of software infrastructure and practice (e.g., security, account management, access, isolation, experiment management, etc.) ?

On the "social" side

Slight cultural changes in our relation to publication and daily practice

- Changing our social model to favor adoption of better practice
  - Artifact evaluation, open reviews, ... (e.g., IPOL, ReScience)
  - Alternative evaluation models (publishing, funding, ...)
- Learning is the essence of our work. $\rightsquigarrow$ Train our researchers and students
  - MOOC on Reproducible Research in Oct. 2018 on FUN
  - Train in statistics, experimental practice, design of experiments

It's up to us. **We** should **care** and **take the lead**

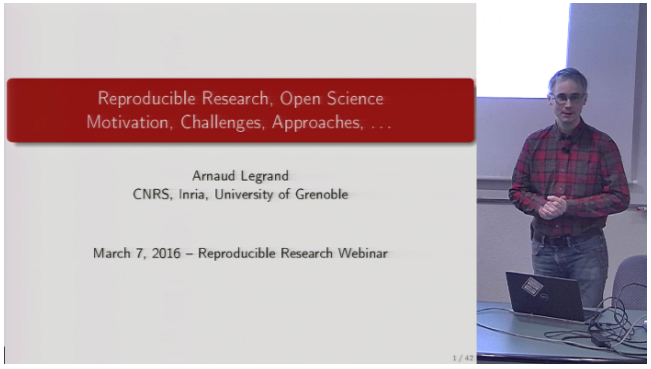
Main benefit:

- Higher confidence in our work $\rightsquigarrow$ definite competitive advantage
- Our research becomes sound, deeper, auditable, more visible, reusable

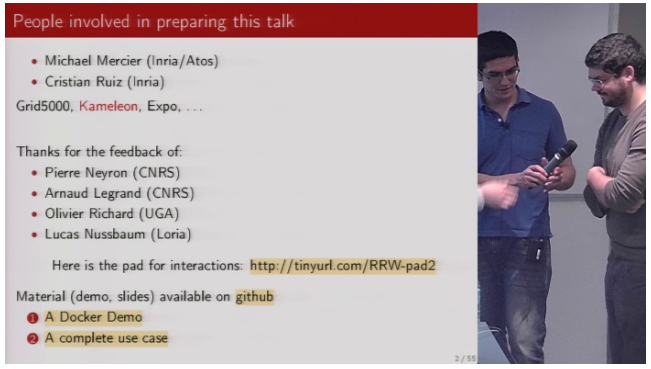
Webinars: Learning by Doing

Many different tools/approaches developed in various communities

1. Replicable article
2. Logging your activity
3. Logging and backing up your data
4. Organizing your data
5. Mastering your environment
6. Controlling your experiments
7. Making your data/code/article available
8. Publication modes
9. Artifact Evaluation



Litterate programming



Controling your environment

Numerical reproducibility

Logging and backing up

https://github.com/alegrand/RR_webinars