

# SCIENTIFIC METHODOLOGY AND (EMPIRICAL|EXPERIMENTAL) EVALUATION

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Master 2 MOSIG  
2023-2024



# OVERVIEW

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# TEACHERS AND CONTACT



## Resources

- Github (schedule, slides, homeworks)
- MOOC (Learn reproducible research by yourself)

## Communication

- Pad (notes and homework reporting)
- Mattermost (questions, references, ...)

# QUICK POLL

- Python
- R
- Notebooks (Rstudio, Jupyter, Org-Mode)
- Git
- Docker
- Confidence Interval
- P-value, P-hacking
- Linear regression
- Model Selection
- Design of Experiments
- Reinforcement Learning

# TENTATIVE SCHEDULE

12 lectures    Many practical homeworks (50%)    A final Exam (50%)

1. Epistemology: scientific method and computer science    Presentation of the lecture
2. Visualization and Exploratory Data Analysis    Correlation/causality, spurious correlation
  - No lecture
3. Data curation with the tidyverse    Beautiful Viz with ggplot
4. Data management: theory    Data management: tools
  - Fall Vacations
5. Measurement and tracing
6. Clearly defining the experiment    Having the right tools to analyze (e.g., C.I)
7. The linear model
8. Multiple testing, ANOVA, and p-hacking
9. Scientific integrity
10. A Bayesian perspective on model selection    Sequential DoE (screening, LHS, D-opt, ...)
11. Ethics (AI and human, climate change, societal challenges)
  - Winter vacations
12. Incremental DoE: Bayesian perspective, Reinforcement Learning, Surrogates (Bandit, GP)
  - Exam

# TOWARDS A RIGOROUS AND ETHICAL COMPUTER SCIENCE

## (Computational) Reproducible Research

- Journal and computational notebooks
- version control
- Containers

MOOC

## Observation vs. Experiments

- Measurement / Tracing
- Modeling (parameters)
- Planning and Design of Experiments

## Statistics

- Confidence interval and p-value
- Linear model and model selection
- Frequentist vs. Bayesian
- Test and inference

## "Meta" Science

- Epistemology
- Scientific Integrity (fraud & errors)
- Publication, evaluation, and credit
- Ethics

## Data Management

- DMP, license
- File organisation, metadata
- version, archiving

## Data Analysis/Visualization/Presentation

- R (python)
- Tidyverse (dplyr, ggplot)

MOOC



# REPRODUCIBLE RESEARCH

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# SCIENTIFIC CONSENSUS

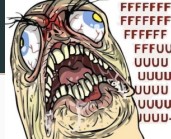




# NO TRANSPARENCY NO CONSENSUS



# COMMON HORROR STORIES 1/3: *WHAT DID I DO?*



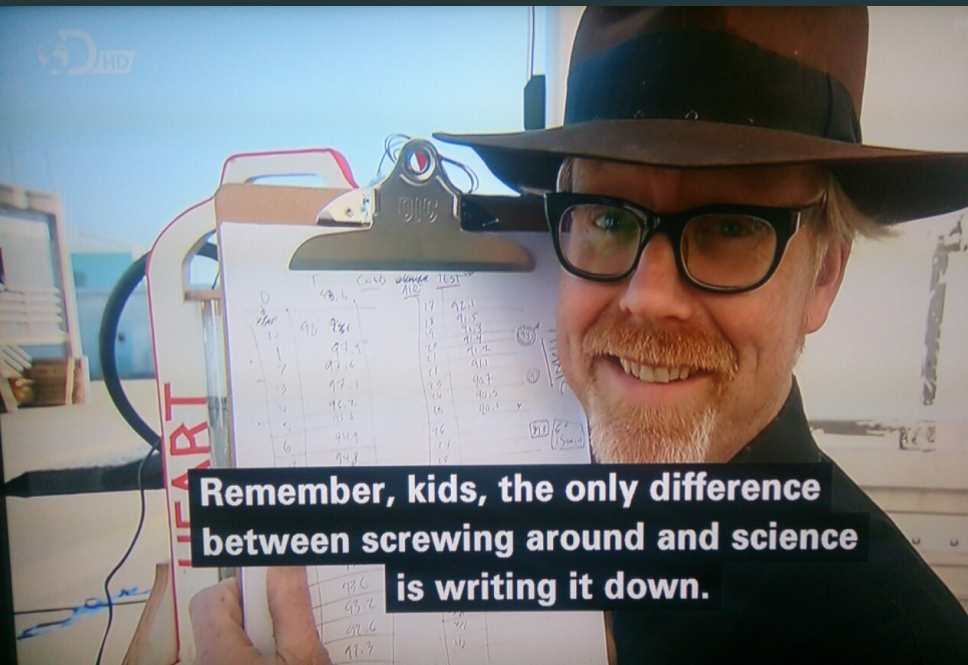
## Author

- 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?

## Reviewer

- 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

## MYTHBUSTERS: SCIENCE VS. SCREWING AROUND



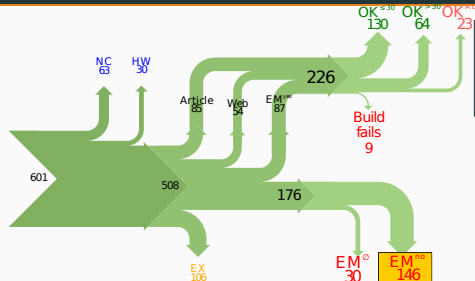
**Remember, kids, the only difference  
between screwing around and science  
is writing it down.**

## COMMON HORROR STORIES 2/3: ARGH... DAMNED COMPUTERS

- **Alice:** I got 3.123123                      **Bob:** I got segfault
- Damned! It used to work!!! Whenever I upgrade my computer, things break so I try to stay away from this 😞
- Whenever trying the code of my colleague, I had to install Foo but I broke everything and now neither his code nor mine works! 😞
- But hey! Here is my code. It's on GitHub so feel free to play with it! I'm doing open science 😊

Seriously ? It's 21st century. How come all this is so painful ?

# COMMON HORROR STORIES 3/3: PLEASE HOLD ON



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

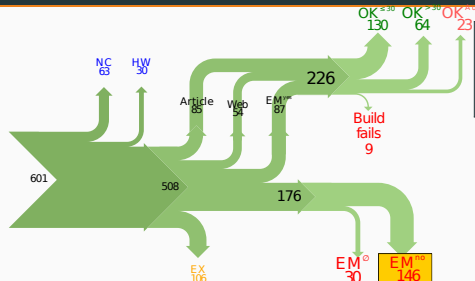
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- $EM^{no}$  = the code cannot be provided
- Versioning Problems

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*



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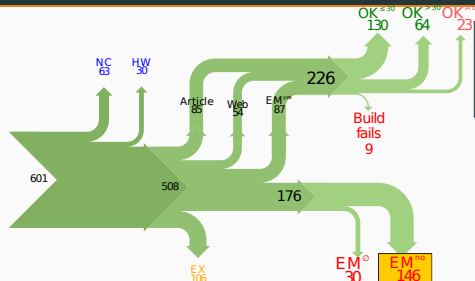


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- EM<sup>no</sup> = the code cannot be provided
- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon

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.

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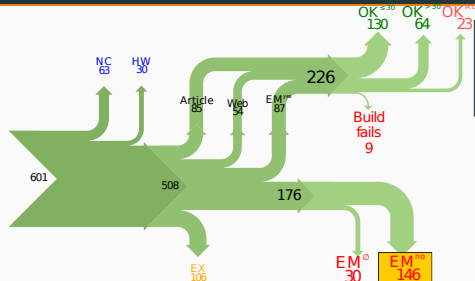
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- Code Will be Available Soon
- No Intention to Release

*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.*



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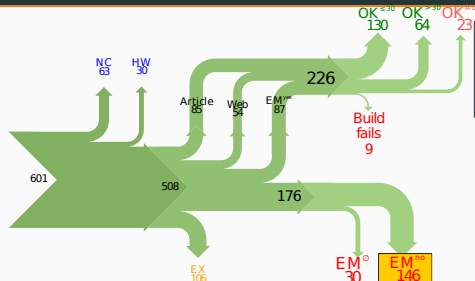
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*<STUDENT> was a graduate student in our program but he left a while back so I am responding instead. For the paper we used a prototype that included many moving pieces that only <STUDENT> knew how to operate and we did not have the time to integrate 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*

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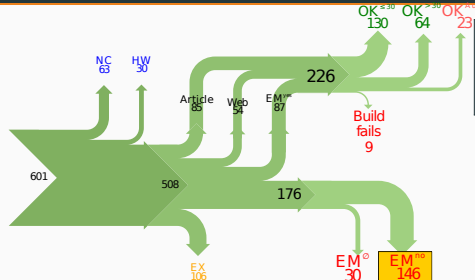
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  - Programmer Left
  - Commercial Code
- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release

Since this work has been done at  $\langle \text{COMPANY} \rangle$  *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*  $\langle \text{COMPANY} \rangle$ , and AFAIK the code is not open-source. Your best bet is to reimplement :( Sorry.

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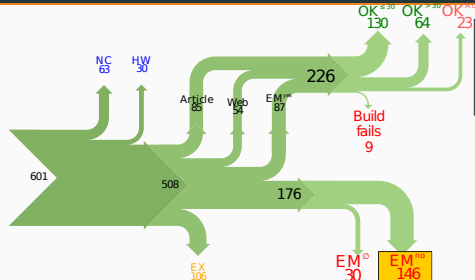
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- EM<sup>no</sup> = the code cannot be provided
- Programmer Left
- Commercial Code
- Proprietary Academic Code

Unfortunately, the  $\langle \text{SYSTEM} \rangle$  sources are *not meant to be opensource* (the code is partially *property of*  $\langle \text{UNIVERSITY 1} \rangle$ ,  $\langle \text{UNIVERSITY 2} \rangle$  and  $\langle \text{UNIVERSITY 3} \rangle$ .)

If this will change I will let you know, albeit I do not think there is an intention to make the  $\langle \text{SYSTEM} \rangle$  sources opensource in the near future.

If you're interested in obtaining the code, *we only ask for a description of the re-*<sup>9/13</sup>

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- $EM^{no}$  = the code cannot be provided
  - Programmer Left
  - Commercial Code
  - Proprietary Academic Code
  - Research vs. Sharing
- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release

*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.*

# DIFFERENT REPRODUCIBILITY CONCERNS IN MODERN SCIENCE

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

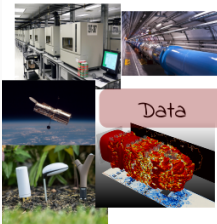
**Genomics** software engineering, computational reproducibility, provenance

**Computational fluid dynamics** numerical issues

**Artificial Intelligence** most of the above

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

Authors



Data

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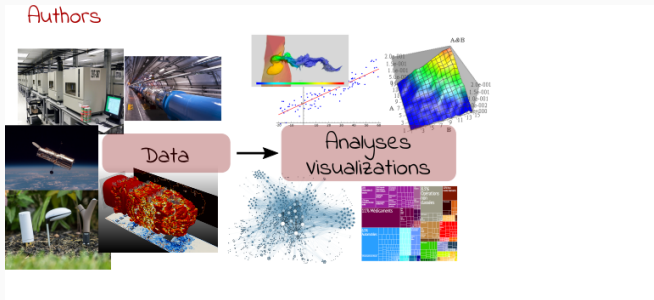
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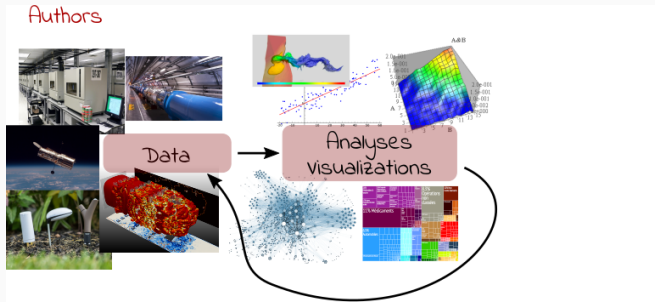
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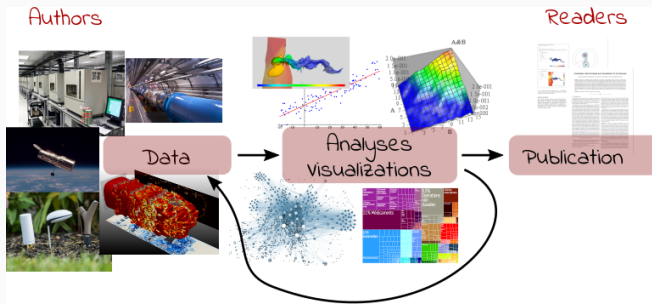
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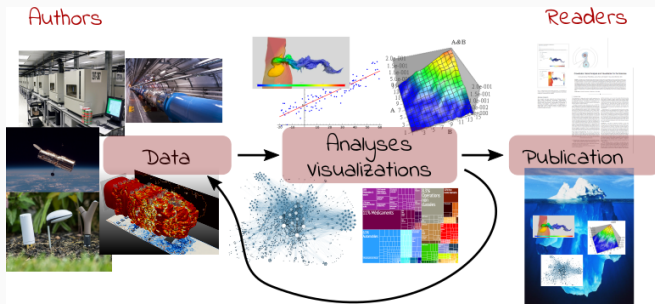
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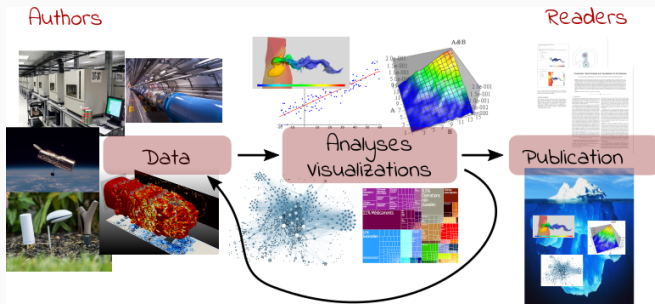
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Reproducible Research = Bridging the Gap by working Transparently 10/13

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

**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



**Learn and Teach** using online resources like

- **Software Carpentry**, **The Turing Way**, ...

# THE REPRODUCIBLE RESEARCH MOOC

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

- Konrad Hinsen, Christophe Pouzat
- **3rd Edition**: March 2020 – March 2023 (15,000+)
- In French but fully subtitled in English



**Module 1** Taking notes (markdown, git)

**Module 2** Computational document (Jupyter, Rstudio, Org-Mode)  
*Data Analysis of the Space Shuttle: Pre-Challenger Prediction of Failure*

**Module 3** Reproducible analysis

Data analysis : 7 possible subjects and a Peer evaluation

**Module 4** Reproducibility Pitfalls (Hell)

Stay tuned for the **MOOC "Advanced RR"** planned for 2021 2022 2023

- Managing data
- Software environment control
- Scientific workflow

# HOMEWORKS

- ☐ Read Popper's text
- ☐ Indicate your name on the Pad.
- ☐ Register on the Mattermost.
- ☐ Set up a **public** github or gitlab project for this lecture.
- ☐ Register to the MOOC
- ☐ Follow modules 1 + 2 of the MOOC with as much exercises as possible
- ☐ Set up a computational document system (e.g., Rstudio or Jupyter)
- ☐ Report the URL of your git project, your mattermost ID on the Pad.