University of Basel

HPC Class - Chap 7 - Reproducilibity

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Quick poll (1/2)

Practices

- How are you plotting? Python/Gnuplot/R/...
- How are you running your experiments?
- How are you sharing code/data?
- How are you managing your software environments?
- Do you use notebooks? Jupyter/Rmarkdown/Orgmode/...

Quick poll (2/2)

Never have I ever...

- forgot which parameters I used for an experiments?
- forgot which version of the code I used?
- lost some scripts?
- forgot why I did something several months agos?
- failed to re-run something I did several months ago?

Introduction

The Reproducibility Crisis

- Baker [1], [2] raised awarness about the issue
- since then all the fields of science are getting concerned/interested in repro

What is "Reproducibility"?

- It depends who you ask .... No consensus between sciences
- In computer science: ACM gave some definitions [3]
  - *Repeatability* (Same team, same experimental setup)
  - *Reproducibility* (Different team, same experimental setup)
  - *Replicability* (Different team, different experimental setup)
- some sciences use also the term "Robustness"

What is the goal of Reproducibility?

- should not all research work be reproducible?
- is it a proof of the correctness of the work?
- restore trust in science
- or an effort so that future researchers can use the work?
  - *"Standing on the shoulders of giants"*
  - the objective: ✨ precise introduction of Variation ✨

Open Science and FAIR [4]

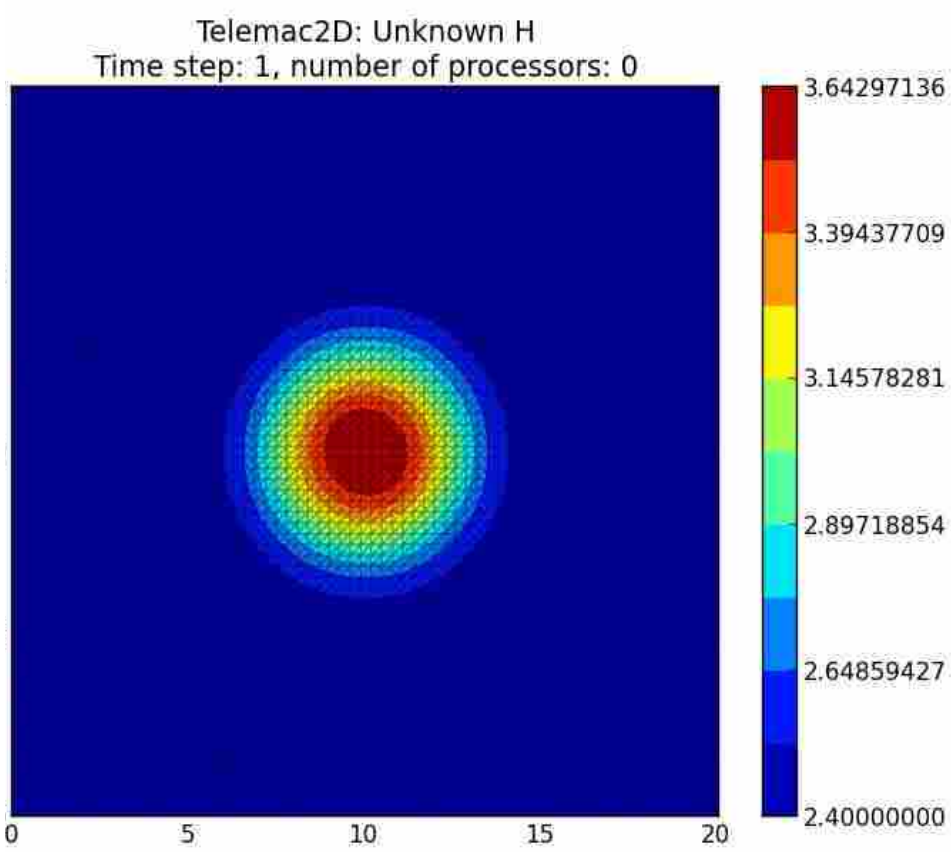
- **F** indable, **A** ccessible, **I** nteroperable, **R** eusable
- Open Science: one key concept is "**Transparency**"

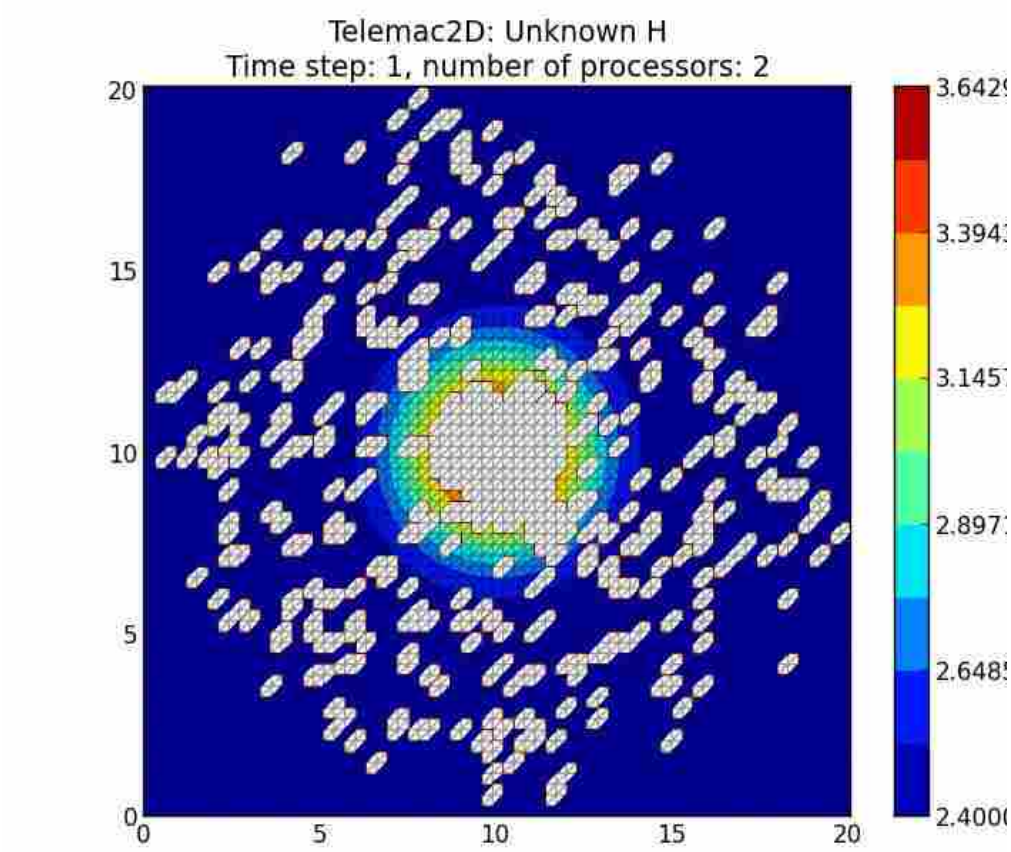
What about in Computer Science?

"Computers are deterministic, hence no reproducibility issues" – a fool

- floating point associativity ($\lfloor a + \lfloor b + c \rceil \rceil \neq \lfloor \lfloor a + b \rceil + c \rceil$)
- order of compilation flags has an impact on the performance
- the size of the environment variable has an impact on performance [5]
- computers are physical machines: heat, noise?! 📽️
- Experiments are *"quick"* and *"free"* ⟶ leads to some quick and dirty work
- Programming errors, mistakes (Excel 🤡 [6])
- How to compare 2 solutions?
- many more...

Simulation of a drop of water [7]





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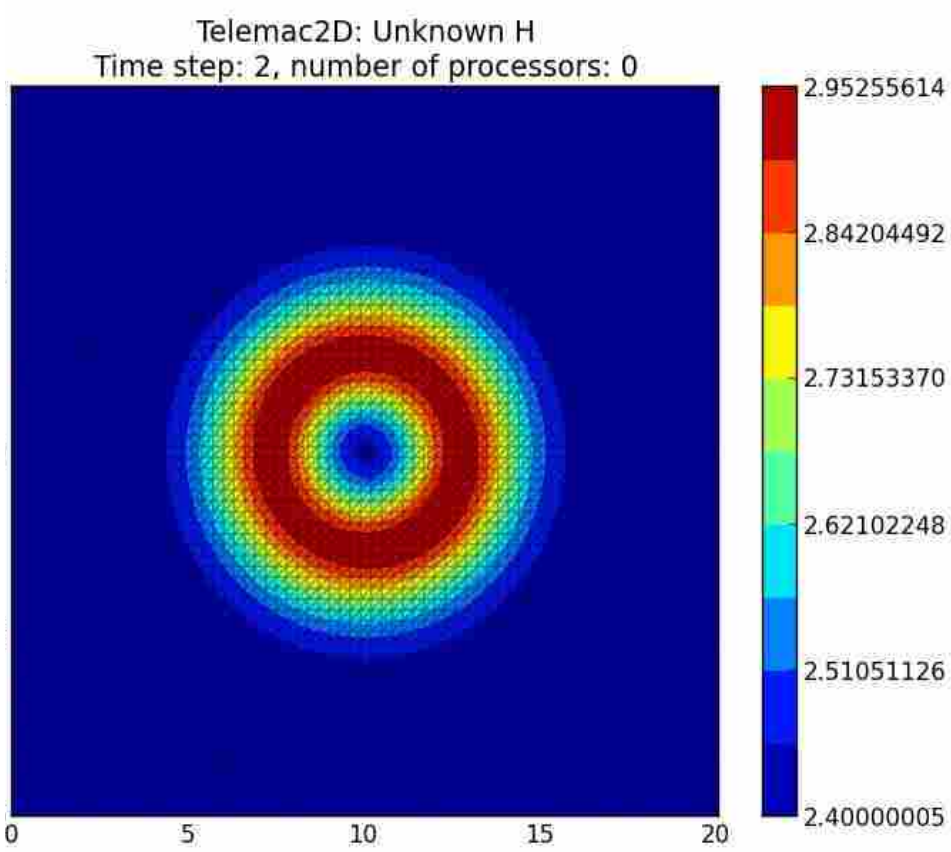

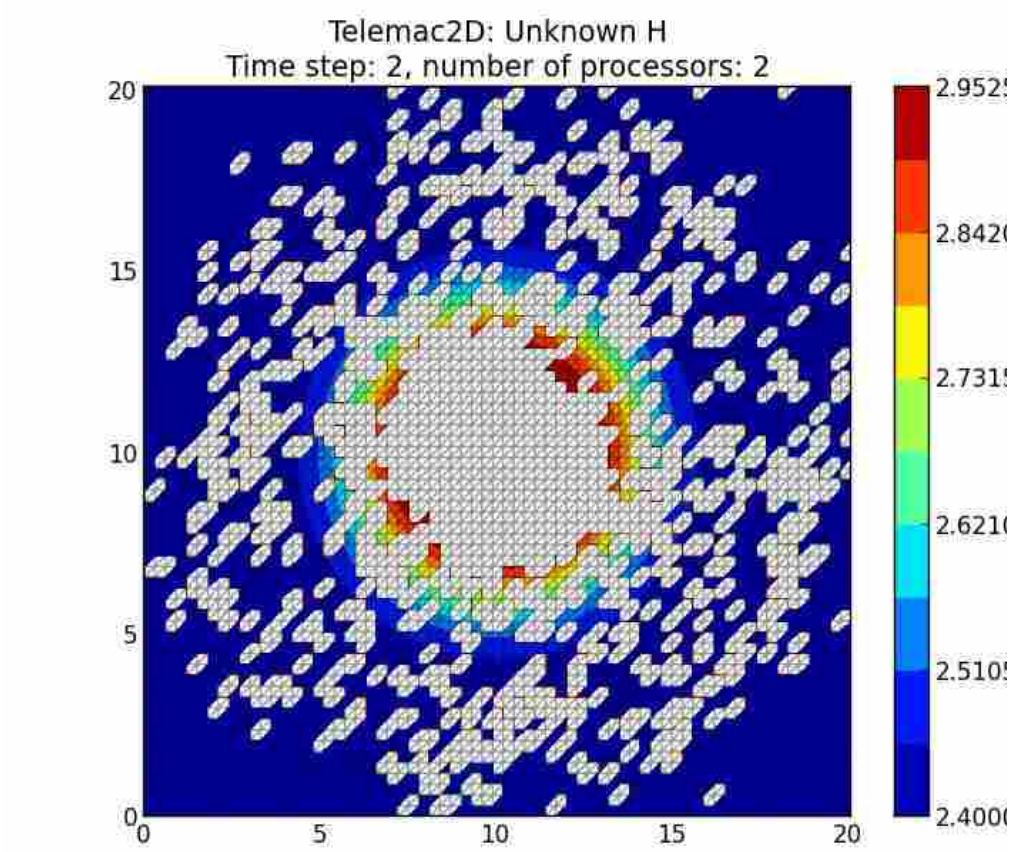

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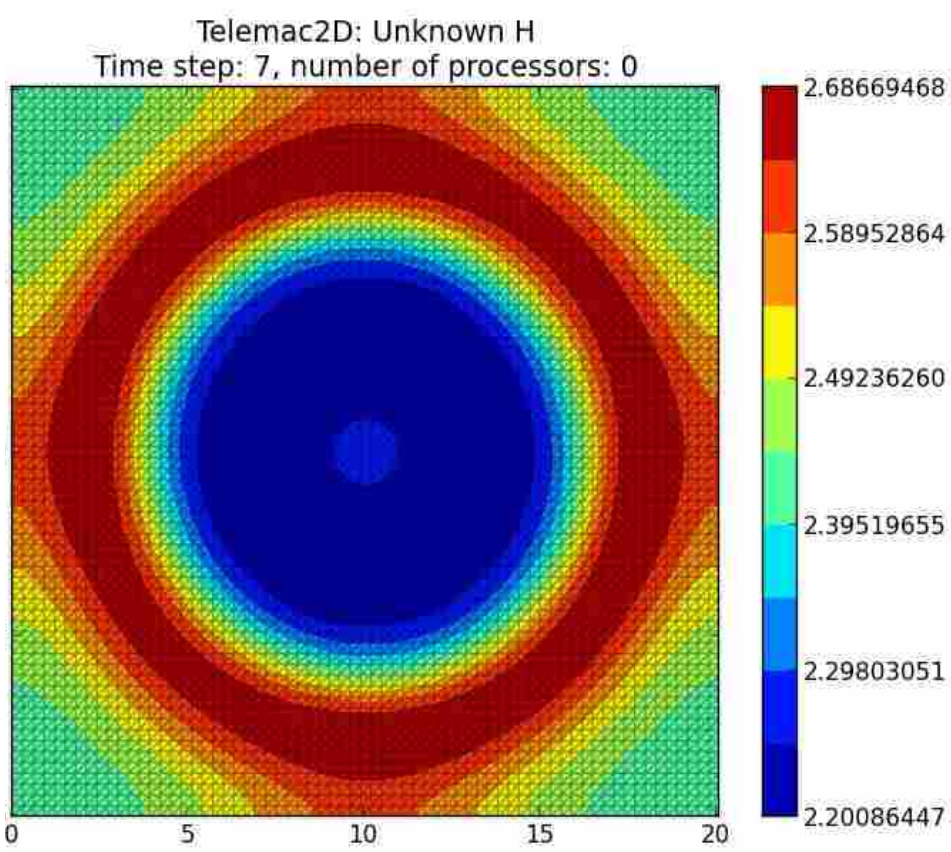

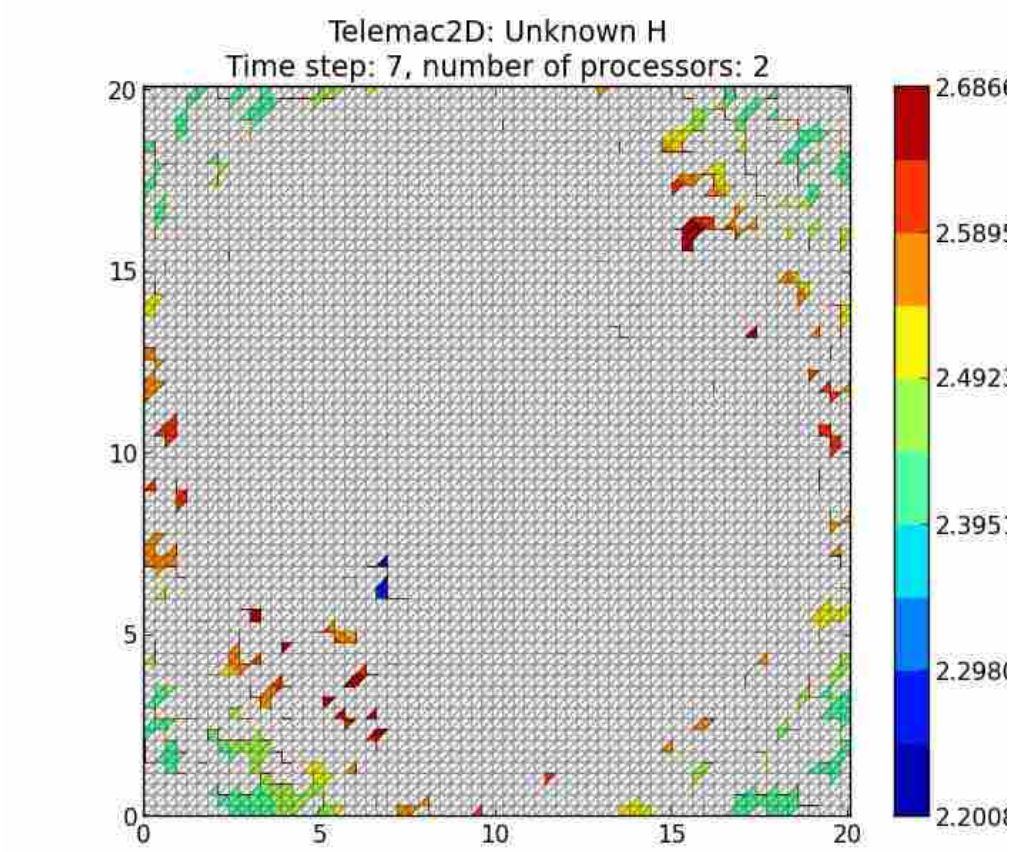

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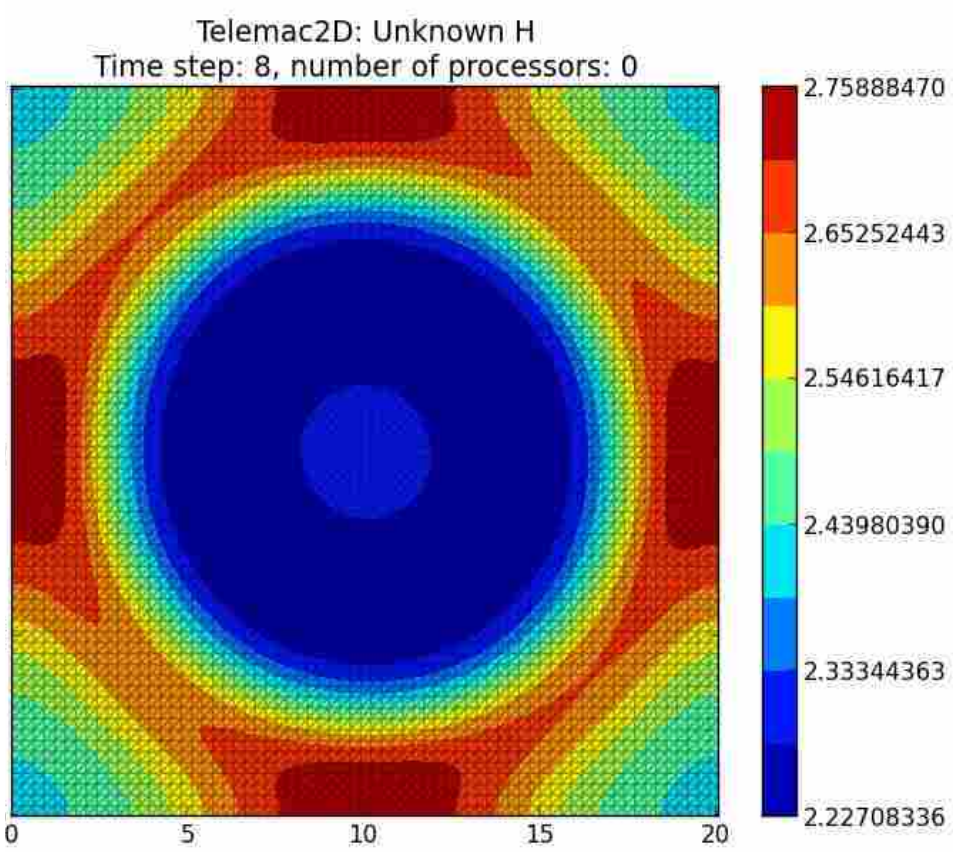
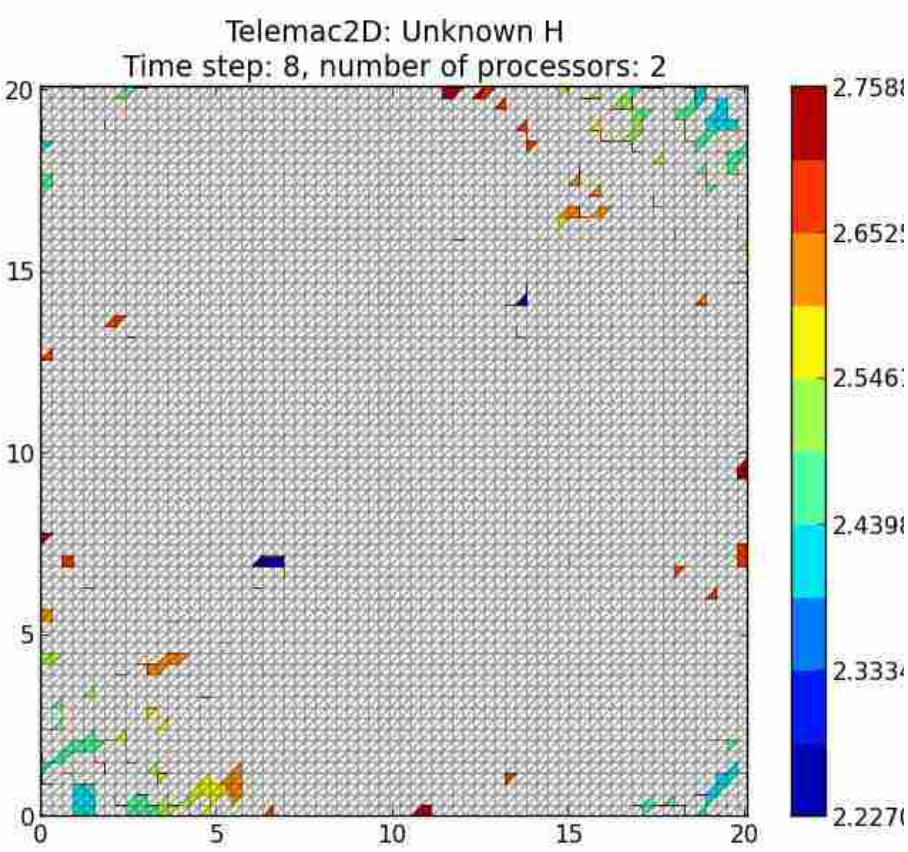


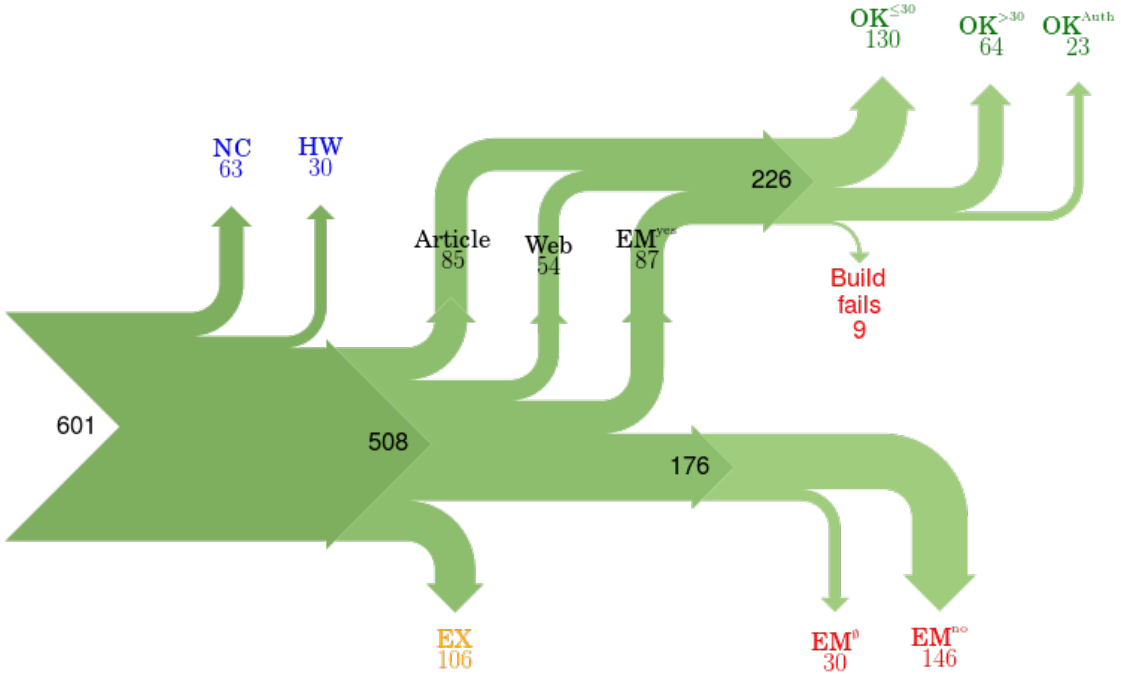


What does the community think?

- Hunold [8] : Surveyed the HPC community in 2015
  - 94% think the state of reproducibility needs to be improved
  - 58% think that 10% of the papers in HPC are reproducible
  - why not sharing code/data/scripts?
    - 84% to retain a “competitive” advantage
    - 87% it is not rewarding
    - 90% irrelevant because evolution is too fast
  - 42% think that their own work are mostly not reproducible

"My dog ate my code"

- Collberg et al. [9] (2015)
- looked at 600 papers and try to get the code and reproduce the results
- and contacted the authors
- funny responses from the authors



Some answers

"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****. So, I cannot really guarantee that you will enjoy playing with it."*

"⟨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"*

"Most importantly, ***I do not have the bandwidth*** *to help anyone come up to speed on this stuff."*

Some recent findings

Artifact Evaluation

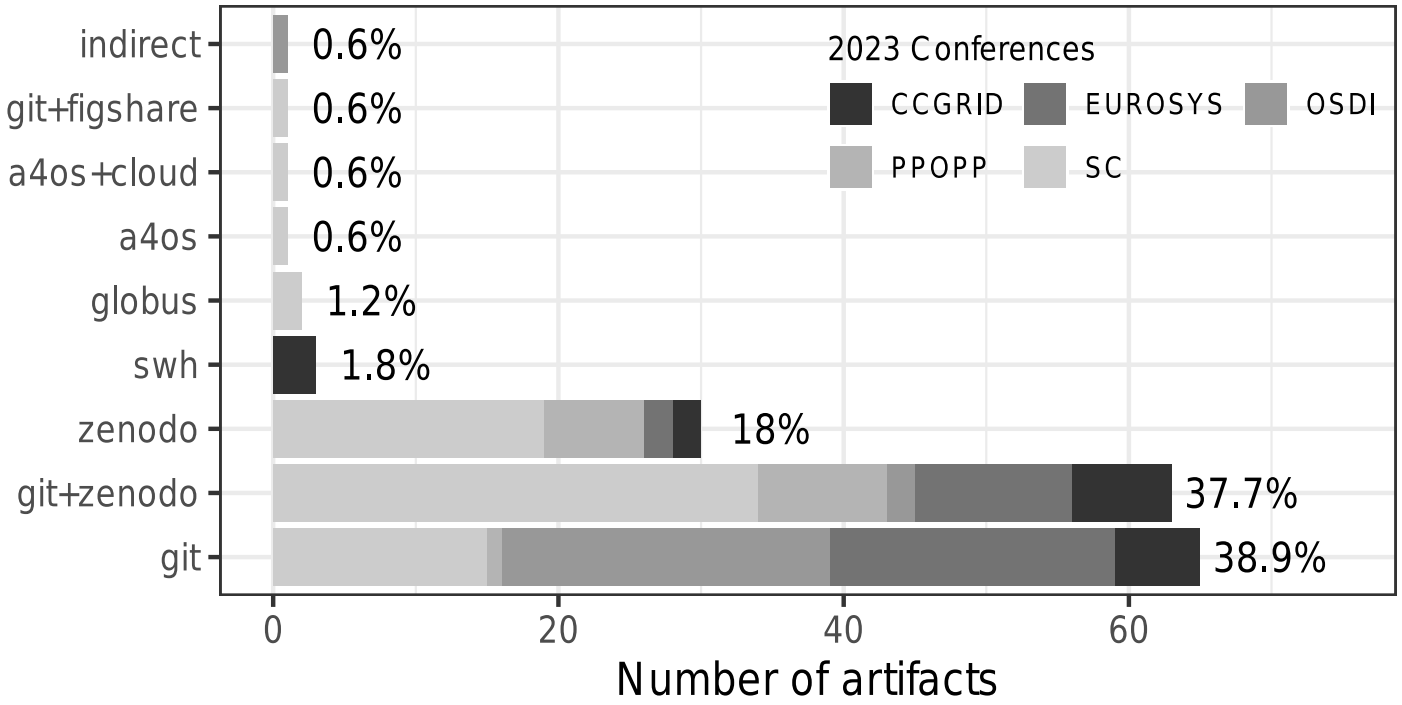
- Conferences and journals are now having an "Artifact Evaluation" process to make sure that the accepted papers are "reproducible"
- Authors send their code, scripts, data and a description of how to use it
- then reviewers will try to rerun experiments

- the goals:
  - validate results
  - restore trust
  - promote artifact sharing

How are authors sharing their artifacts?

- Guilloteau, Ciorba et al.
- Looked at 5 *top conferences* of 2023 in HPC/distributed systems
- 296 papers in total
- 157 had an artifact description
- 101 had the top badge
- 168 URLs to code in the papers
- 154 URLs valid at the time of the study

Sharing the code/data



- mostly just a Git(Hub|Lab) URL and/or a Zenodo archive

The worst case scenario

What if GitHub closes? What if the authors delete the repository?

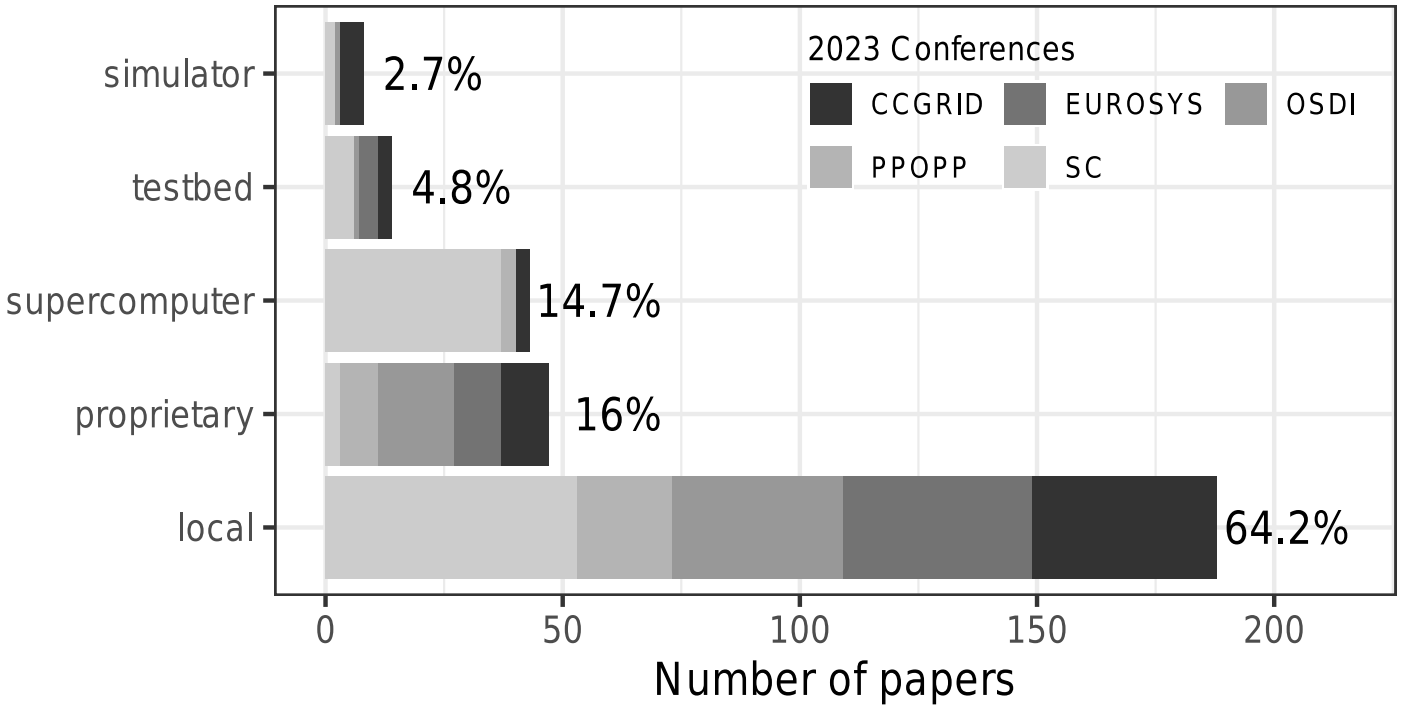
"Bah! GitHub will never close!" (😬 Google Code, Forge Inria)

Can you imagine if the proof of a math paper disappears? (Fermat 🙃)

Recommendation for long term archiving:

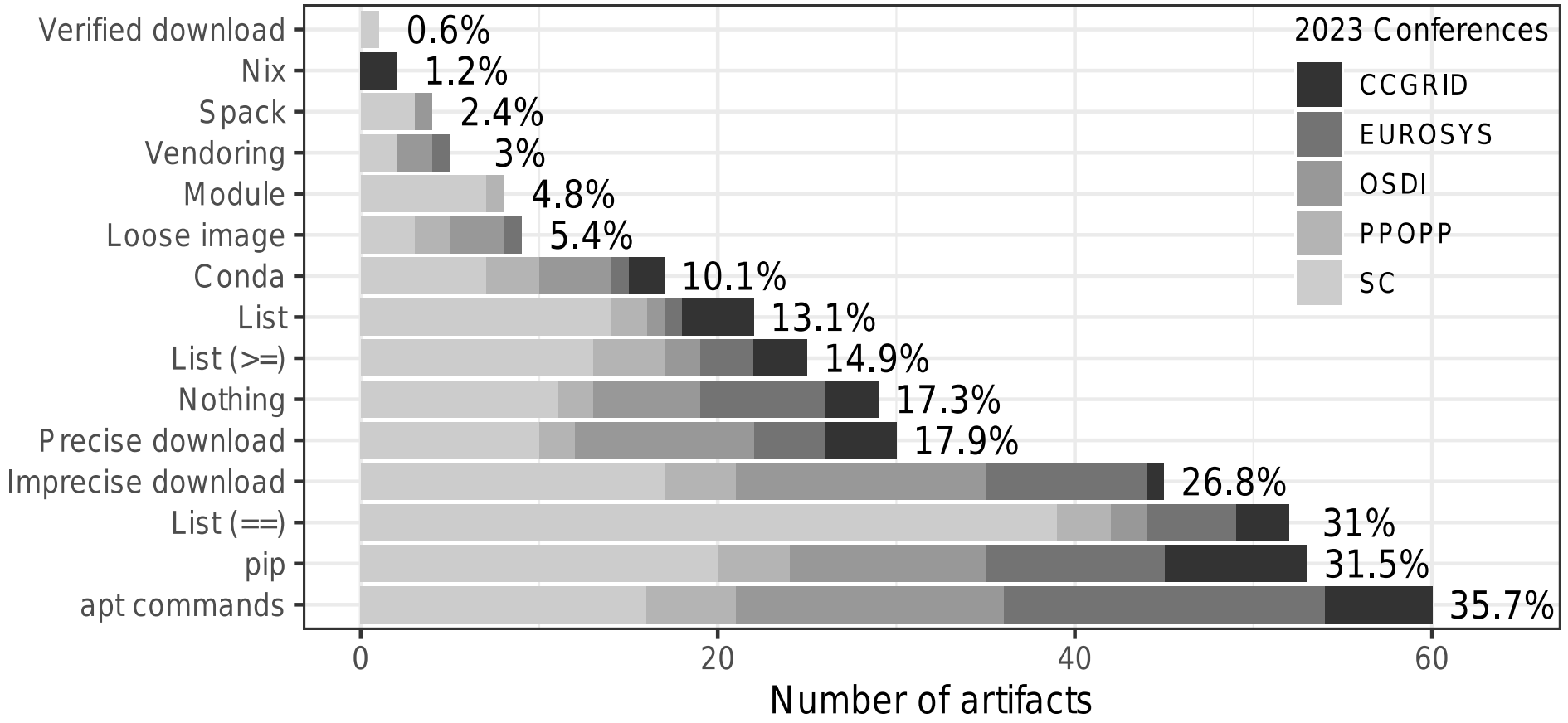
- For source code: Software Heritage (UNESCO) 
- For data: Zenodo (CERN)

Where are the experiments done?



- How to get access to **those** machines? → Azure/AWS/Google Cloud .... 💸

How is the software environment captured/described?



Some software environments problems

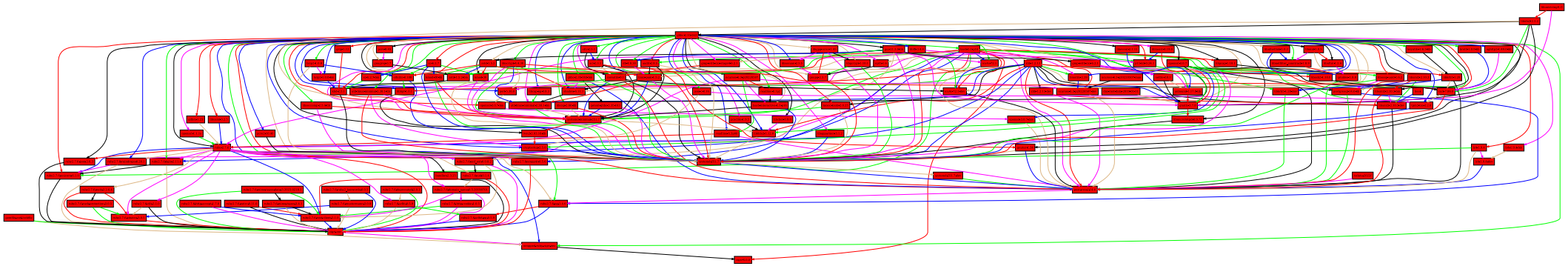
- **requirements.txt** → what about the **other** dependencies?
- List of packages (**apt install**) → what if forgotten packages? install **specific** version?
- Module → what is their lifetime? how to share? how to modify?
- Virtual Machines and Containers
  - Binary format → no transparency! → better: the recipe (e.g., Dockerfile)
  - Container → what about the OS/Kernel/Drivers ?
- Spack ? → better but not (totally) reproducible
- Perennity of the shared artifact?
- Non-free software?

What is wrong with this Dockerfile?

```
FROM ubuntu
RUN apt-get update -y && \
    apt-get install -y \
     build-essential\
     ...\
     simgrid
RUN git clone https://github.com/JohnDoe/chord.git
WORKDIR chord
RUN curl -L https://tinyurl.com/patchchord -o increase-timeout.patch
RUN git apply increase-timeout.patch
RUN cmake .
RUN make
ENTRYPOINT ["./chord"]
```

What a "complex" software environment looks like

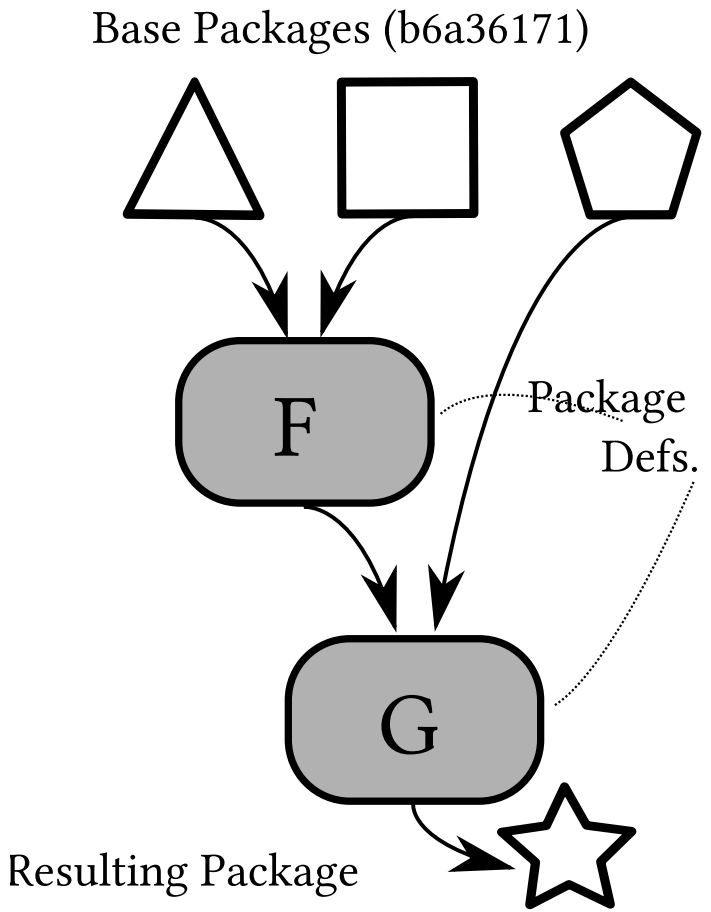
CiGri: a single component of the system during my PhD



How to manage such software environments in a *reproducible* way?

Functional Package Managers

- Nix [10], Guix [11]: reproducible by design!
- packages = functions
  - inputs = dependencies
  - body = commands to build the package
- sandbox, no side effect
- **/nix/store/hash(inputs)-my-pkg**
- immutable, read-only
- precise definition of $PATH
- can build: container, VM, etc.



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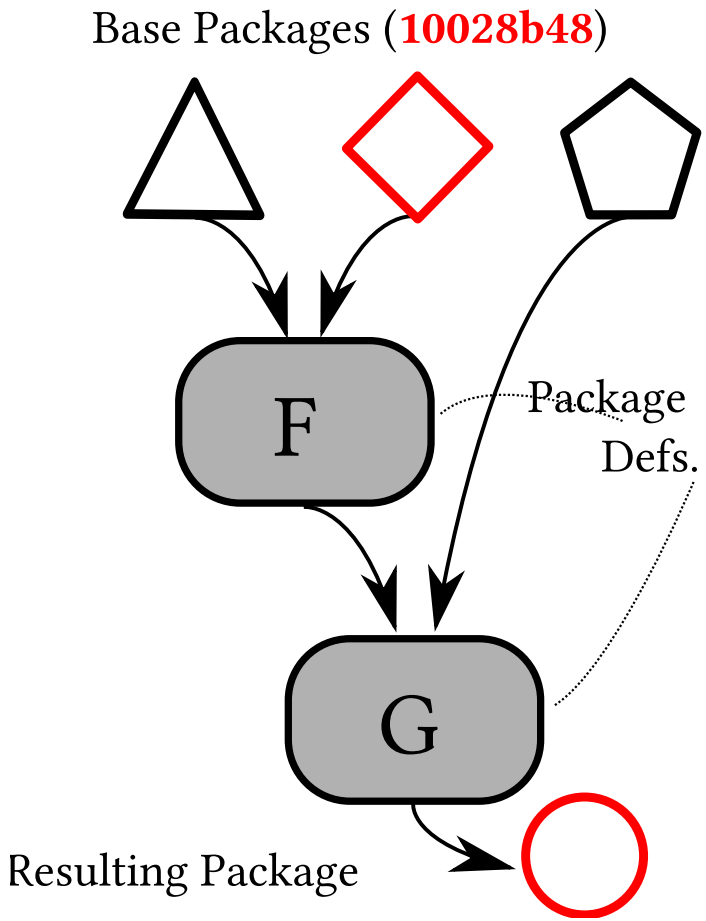

Workflow

Doing experiments

Never do experiments by hand

Doing experiments

NEVER do experiments by hand

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State of the Practice

The state of the practice:

copy-paste commands from a readme or long bash scripts 😬

- error-prone
- not robust
- not extensible
- not scalable

Then what to use?

✨ Workflow Managers ✨

Workflow Managers

- For example: Snakemake [12], Nextflow [13]
- Like Make, but better
- express the workflow as **rule**s that take **input**s and give **output**s
- manages the dependencies
  - if an input is updated, will re-run everything that depended on this input, and so on
- great expressiveness
- scalable, integration with SLURM, K8S, etc.
- shareable (CWL)
- extendable

An example

Scenario

- parallel matrix multiplication code
- several input matrices
- several number of threads
- several scheduling strategies (LB4OMP)

```
rule expe:
  input:
    bin="my_mat_mult",
  output:
    "data/{matrix}/{sched}/{nb_threads}/{iter}.csv"
  shell:
    "OMP_SCHEDULE={wildcards.sched}\
     OMP_NUM_THREADS={wildcards.nb_threads}\
     {input.bin} {wildcards.matrix} > {output}"
```

→ “I want **data/webbase01/VISS/20/1.csv**”

Conclusion

Checklist for your future

- Use Git
- Do not be shy to share everything (code, data, metadata)
- Automatize as much as possible
- Pay attention to your plots 
- Pay attention to your statistical analysis
- Benchmarking crimes [14]
- Statistical dances 

Conclusion

- Reproducibility is gaining in importance in the scientific community
- Computer Science and HPC are also victims
- The state of the practice is not good enough!
- It is also **your** role to educate your peers on these problematics
- Machine Learning? 🎥

MOOCS:

- MOOC RR1 📚
- MOOC RR2 📚 (starting in a few days)

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What about the environmental cost of Reproducibility?

Next week (2nd of May)

Ch.08 Performance engineering by Jonas Müller Korndörfer

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