

Development Efforts towards Reproducible Research: Feedback and Perspectives

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Overview

1. Introduction

1.1 Definitions of RR

1.2 Motivation

1.3 Implementation of RR, Why RR

2. Efforts on Software Useful for Reproducible Research

2.1 Updated Preview of Reproducible Research Platforms

2.2 Library Development for RR

3. Advanced Editorial Efforts

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3.3 Reviewing process for RR

4. Conclusion

1. Introduction

1. Introduction: some definitions¹

Repeatability and replicability

Capacity to perform the same experiment as many times as needed.

→ **Repeatability:** Same team, same experimental setup

→ **Replicability:** Different team, same experimental setup

Example: is distilled water electrically conductive? Is salt water conductive? We can perform the experiment many times and get results (<https://www.dailymotion.com/video/x21cg6a>).

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Reproducibility

Capacity to obtain the same results when repeating an experiment by following a detailed procedure

→ Different team, different experimental setup

In computational sciences (deterministic code, digital data): results obtained by following a detailed and correct pseudo-code description must coincide if the same input data is provided.

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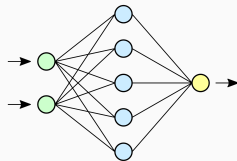
1.1 Definition: Repeatability Examples

Repeatable

Obtaining the classification results with a **neural network**.

We can **repeat** the experiment as many times as we want.

We just need the weights of the network and the input data.



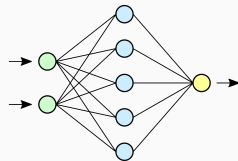
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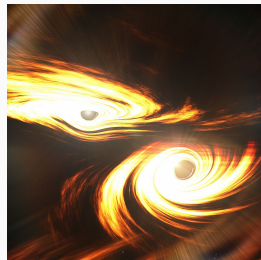
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Not repeatable:

Detection of the merger of two black holes from gravitational waves. We can't repeat the experiment as needed.



1.1 Definition: Reproducibility Examples

Reproducible:

Given:

- a detailed pseudo-code (or the source code itself),
- any associated learning or initialization data,
- the input data,

we should obtain exactly the same results each time we run the algorithm.

⇒ **Exactly the same** denoised image, classification results, etc.

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Not reproducible

In a paper that shows

- a pseudo-code without **all the details**, or its **initialization**,
- the source code is not available,
- neither the learning data,

other researchers **can't compare** with the proposed method.

⇒ We can't be sure about anything on the method, nor test it with **their own data**.



1.2 Motivation: Example on Biomedical Research

Main Keys Points

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Sources:

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- **Bayer HealthCare Germany** confirmed: only **25%** of cancer research is reproducible.

Source: <https://www.nature.com/articles/nrd3439-c1>

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- Computational sciences: **no excuse!**

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Several reasons in general:

- Some researchers don't want to **make public working code**
 - doesn't correspond to any version of the pseudo-codes,
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 - quality software takes more time to produce: testing, documentation, objective quality metrics, ...
- Results of a method **do not generalize**
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Not really considered for career advance

- Classic metrics: "number of high impact-factor classic publications"
- Software is considered as a 2nd class citizen

Good news:

The French government is promoting a Plan for Open Science

- <https://www.ouvrirelascience.fr/second-national-plan-for-open-scienc>
- "Path three: opening up and promoting source code produced by research"
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Initiatives at European level

- European Open Science Cloud (EOSC): recommendations to the European Commission
<https://www.eosc.eu>
- Publication: "Scholarly infrastructures for research software"
<https://op.europa.eu/en/publication-detail/-/publication/145fd0f3-3907-11eb-b27b-01aa75ed71a1/language-en>

2. Efforts on Software Useful for Reproducible Research

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2.1 Updated Preview of Reproducible Research Platforms

- Synthetic recall of main platforms [\[CKK19\]](#).
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2.2 Library development

- Another ways to help for RR.
- Examples of library efforts from image domains.

2.1 Updated Preview of Reproducible Research Platforms

Different types of platforms [CKK19]

- Online execution platforms.
- Dissemination platforms.
- Peer-reviewed journals.

- **Galaxy** - <https://galaxyproject.org>
- **IPython** - <https://ipython.org>
- **Jupyter** - <http://jupyter.org>
- **RunMyCode** - <http://www.runmycode.org>
- **Code Ocean** - <https://codeocean.com>
- **DAE** - <http://dae.cse.lehigh.edu/DAE>
- **IPOL** - <https://www.ipol.im>
- **Research Compendia** - ResearchCompendia.org
- **MLOSS** - <https://mloss.org/software>
- **DataHub** - <https://datahub.io/>
- **PaperWithCode** - <https://paperswithcode.com>

- **ReScience Journal** - <http://rescience.github.io>
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- **IPOL** - <https://www.ipol.im>
- **Research Compendia** - ResearchCompendia.org
- **MLOSS** - <https://mloss.org/software>
- **DataHub** - <https://datahub.io/>
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New Reproducible Research Platform (1)

Platform <https://reproducedpapers.org>

[Dissemination platforms]

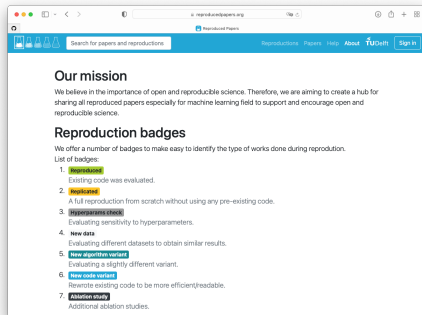
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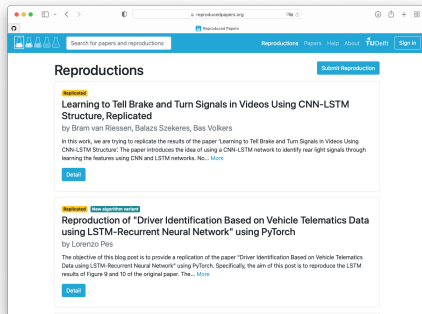


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New Reproducible Research Platform (2)

Platform <https://replicability.graphics>

[Dissemination platforms]

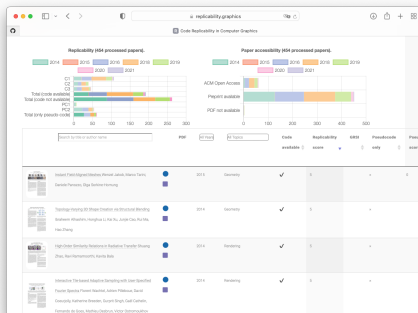
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- Replicate and evaluate difficulty to reproduce SIGGRAPH papers.
- Light formatted review rating the success of replication.

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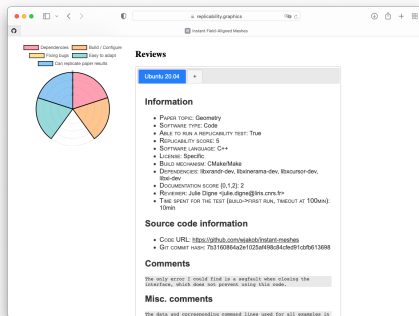


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ReproZip: <https://server.reprozip.org>

[Online execution platforms]

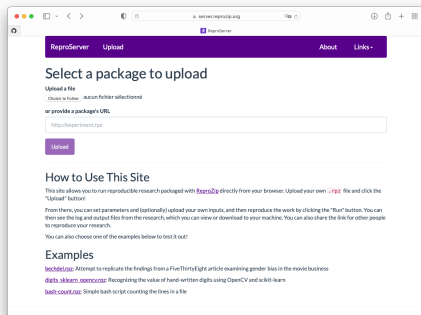
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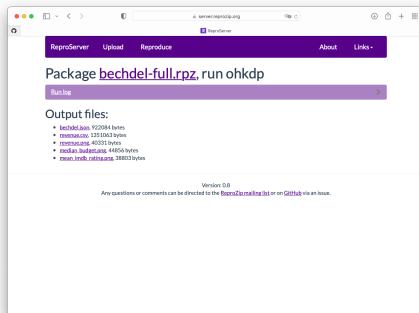


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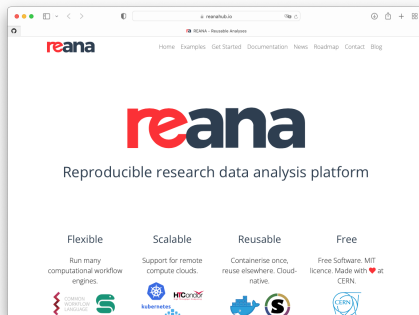


New Reproducible Research Platform (4)

Platform **REANA** : <https://reanahub.io>

[Online execution platforms]

- Reproducible research data analysis platform.

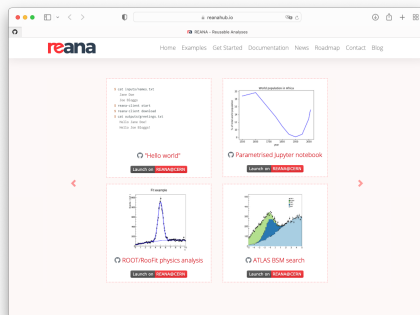


New Reproducible Research Platform (4)

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- Reproducible research data analysis platform.
- Allow to launch workflows from external sources (GitHub, GitLab).

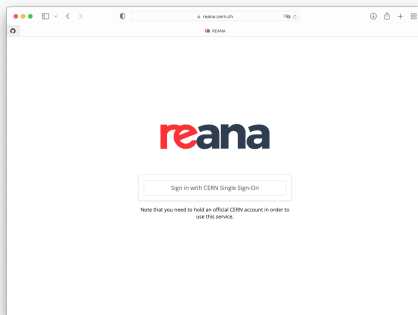


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[Online execution platforms]

- Reproducible research data analysis platform.
- Allow to launch workflows from external sources (GitHub, GitLab).
- Reserved to CERN members only.
⇒ limited impact



New Reproducible Research Platform (5)

Platform <https://replicate.com>

[Online execution platforms]

- Machine learning code replication.
- Applying ML from real-world problem without complex code installation.
- Propose model, run online, run with API or from your computer.
⇒ base on COG (open source tool to package a production ready container)
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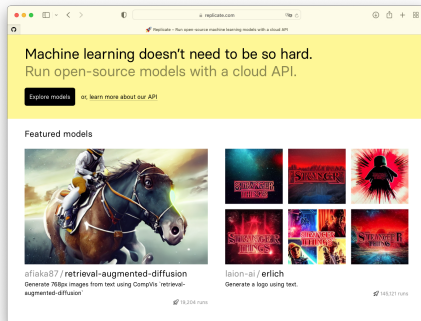
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The screenshot shows a web browser displaying the Replicate platform interface for a model named 'nightmareai / disco-diffusion'. The page includes the following elements:

- Model Name:** nightmareai / disco-diffusion
- Public:** Generate images using a variety of techniques - Powered by Discoart
- Stats:** 46,151 runs, GitHub, License
- Navigation:** Overview, Examples, Versions
- Latest version:** 3c128f6249f - pushed 2 weeks, 4 days ago - View version details
- Run Options:** Run model, Run with API (selected), Run on your own computer
- Input Section:**
 - steps:** 250 (Number of steps, higher numbers will give more refined output but will take longer)
 - prompt:** A beautiful painting of a singular lighthouse, shining its light across
 - Text Prompt:**
 - width:** 1280
- Output Section:** A generated image of a lighthouse scene with a red glow.

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The screenshot shows the arXiv page for the paper "Code Replicability in Computer Graphics" by Nicolas Bonneel, David Coeurjolly, Julie Digne, and Nicolas Mellado. The paper is from the Digital Libraries section, submitted on 1 May 2020. The abstract discusses the importance of replicability in research. The page includes a "Submission history" section and a "Bibliographic Tools" section at the bottom. In the "Bibliographic Tools" section, there are four buttons: "BibTeX Tools", "Code & Data", "Demos", and "Related Papers". The "Code & Data" and "Demos" buttons are highlighted with red boxes. Below the "Demos" button, there is a "Replicate (this is Replicate!)" button, also highlighted with a red box.

2.2 Library Development for RR

Contribution to RR from library development

- Way to diffuse research results to larger use.
- Documented and referenced algorithms easy to be used from new Phd student.
- Extend the classic academic results to real applications.
- Gather algorithms and make easier comparisons and use in other context.
- Make easier software demonstrator or online demonstrations.

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Attentive key point towards reproducibility

- **Compatibility problems:** libraries evolve rapidly (compilation issues).
- **Implementation change:** can change numerical results from a version to another.
- Implies the use of container solution like *Docker* to ensure longer terms reproducibility.

2.2 Library Development for RR: examples (1)

Example of library of vision/image/geometry domains

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PCL	[RC11]	Point clouds	C++	1.12.1	464	2010	Willow Garage
CGal	[The22]	Geometry proc.	C++	5.4	123	1996	Acad./GeometryFactory
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Tulip	[Aub04]	huge graph visualiz	C++/Pyt.	5.6.2	9	2001	Acad./private
Vigra	[Vig]	Comp. Vision	C++	1.11	50	2008	Acad.
DGtal	[DGt]	Digital geometry	C++/Pyt.	1.2	27	2011	Acad. / Project
OpenMVG	[MMPM17]	Mult. View Geom.	C++	2.0	86	2013	Acad./Mikros/Foxel
TTK	[TFL ⁺ 17]	Topology ToolKit	C++	1.0	36	2017	Acad. / Project
Higra	[HIG]	Graph analysis	C++/Pyt.	0.6.5	4	2018	Acad. / Project

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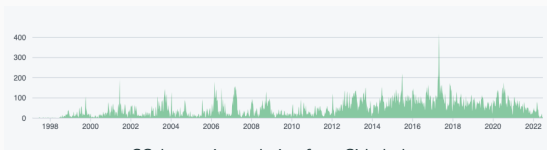
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- The others come mainly from university initiatives.

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Long time efforts

- Commit evolution over 25 years from the CGal library [[The22](#)].

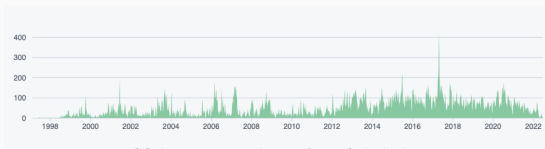


CGal commits evolution from Github data

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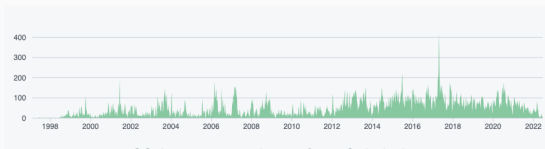


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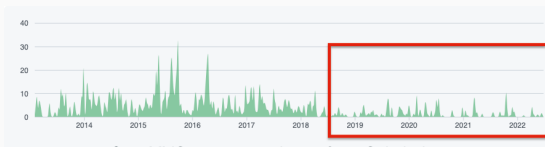
2.2 Library Development for RR: examples (2)

Long time efforts

- Commit evolution over 25 years from the CGal library [The22].
- Commit evolution over 10 years from the OpenMVG [MMPM17].
⇒ no more funding from 2016 (open source only)



CGal commits evolution from Github data



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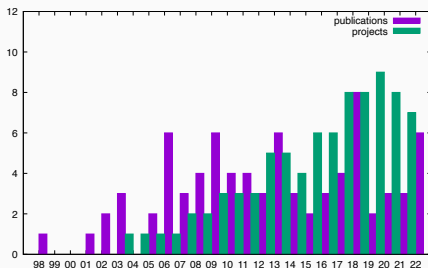
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Example of impact measure

- Geogram library [Geo] (7 authors).
- Estimated from the authors declaring using the library in projects/publications.



2.2 Library Development for RR

Elements to increase reproducibility across libraries

- Limit dependancies to other libraries or include them inside the library itself.
- Orient to an header only library (if C++ like Clmg or CGal since version 5).
- From a user use, extract all dependent header files.

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Examples in C++:

It is possible to use a **special option** in order to list all header files:

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g++ hello.c -o hello -I/specialHeaderLibPath -MD
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Then command will generate a **hello.d** file containing all header files that are really used by the compiler to produce the executable.

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⇒ then an archive can be constructed including only needed files and independently of library or system header file.

3. Advanced Editorial Efforts

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Peer-reviewed

- Both the **article** (PDF) and the **source code**.
- Reproducibility: the reviewers check carefully that the source code matches the pseudo-code.

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Let's have a look! ⇒ <http://www.ipol.im/pub/art/2017/201/>

3.1 IPOL publications: Benefits of RR, from our experience

If a method is worth it, the impact is large

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⇒ other researchers can reuse text, source code, data

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Scientific acceleration:

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Useful for Centre Borelli to show a landscape of our scientific activity

A way of working!

3.2 New initiative with OVD-SaaS

Main idea of the project

- **New long-term project** at **Centre Borelli**
- Inspired on the experience of IPOL
- Opening industrial **software as a service** (SaaS) to **final users**
- Needless to say: based on **reproducible research** and **sharing data**
- Do not focus on technical details of low-level services, but solving a concrete and final **industrial need**

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Even more !

SaclAI-School, MVA track on reproducible research, ...

3.2 New initiative with OVD-SaaS: feedback

Preliminary feedback

- First "ML-Briefs" in April 2022. Second in October 2022.
- Publication of short ML papers.

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Preliminary feedback

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- Publication of short ML papers.
- Some challenges:
 - **Evaluation of neural networks.** They're not "classic" code. Evaluate type of architecture, how the training was conducted (initialization, which datasets. etc). Black-box model to check same outputs.
 - **Instability of libraries.** Use of Python's `venv` not enough. Other dependencies at OS and hardware levels. Using Docker containers.

3.3 Reviewing Reproducible Research: How?

Main attention points:

- Consider **source code** as **part of the publication**, not supplementary material
- Different **levels of evaluation**:
 - **Lowest**: **black box** (same inputs → same outputs)
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Difficulty

- **Software** is **not easy to review**.
- Not all researchers are software engineers!

⇒ A possible solution (IPOL): use **at least two reviewers**, one of them being an expert reading source code.

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Special case of neural networks

Focus on the **architecture**, **training**, **understanding**, and **generalization**.

3.3 Reviewing Reproducible Research: How? (2)

Important point

- **Versioning** is important!
 - Research source code **changes** constantly
 - A publication is steady
- Much of the code is publicly available on platforms such as Gitlab, Github, and others

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Need to identify software artifacts at different levels

- **DOI is not enough:** the pointed object might change (or even disappear!). It's just a **pointer**.
- Need of a **persistent** and **universal archive**
- A good candidate: UNESCO's **Software Heritage** project [\[DCGZ18\]](#)
- **SWHID:** SoftWare Heritage persistent IDentifiers [\[DCGZ19\]](#)
 - **At different levels:** contents, directories, revisions, releases, snapshots
 - Points to **perpetual objects** in an universal archive

A quick review of software and platforms for RR (1)

Scientific Workflows management systems [CBBC⁺17, Hat17]

- **Taverna**: open source scientific workflow management system that provides a workbench for designing workflows, used in **biology, chemistry, meteorology, social sciences**
- **Galaxy**: is very popular workflow system in the **bioinformatics** community and **life sciences**.
- **OpenAlea** is an **open source** scientific workflow system with a **visual programming environment** that enables users to design, execute and interact with workflows
- **Nextflow**: is a **command-line** based workflow system implemented in Groovy (a scripting language for the Java Virtual Machine), developed to **simplify the design of complex parallel scientific workflows**
- **Chimera** system: originated in support of **data-intensive physics computations** as a means to capture and automate a **complex pipeline of transformations** on the data by external software

A quick review of software and platforms for RR (2)

Project/Experiment management systems [Jen22]

- **Neptune**: is a **metadata store** for any **MLOps workflow**. It was built for both research and production teams that run a lot of experiments
- **Weights & Biases**: is a machine learning platform built for **experiment tracking**, **dataset versioning**, and **model management**
- **Comet**: ML platform that helps data scientists **track**, **compare**, **explain** and **optimize experiments** and **models** across the model's entire lifecycle
- **Sacred + Omniboard**: **open-source** software that allows machine learning researchers to **configure**, **organize**, **log**, and **replicate** experiments

A quick review of software and platforms for RR (3)

Project/Experiment management systems

- **Tensorboard**: **visualization toolkit** for TensorFlow
- **Polyaxon**: platform for **reproducible and scalable machine learning** and deep learning applications
- **ClearML**: is an **open-source** platform, a suite of tools to **streamline your ML workflow**
- **Pachyderm**: enterprise-grade, **open-source data science platform** that makes it possible for its users to **control an end-to-end machine learning cycle**
- **MLflow**: **open-source** platform that helps manage the **whole machine learning lifecycle**. This includes experimentation, but also model storage, reproducibility, and deployment

4. Conclusion

4. Conclusions

- **Reproducible research** is needed for the **advancement of science**
- The **article**, the **software**, and **data** **must be all part of the same publication**
- It has a **larger impact**, but it requires a **larger effort** too
- **Researchers need to be rewarded**

4. Conclusions





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- **Researchers need to be rewarded**

Many initiatives on this direction:






- **European:** European Open Science Cloud (EOSC)
- **National:** French *Plan for Open Science*. **Discussion:** others?
- **Centre Borelli:** IPOL, OVD-SaaS, MVA track on reproducibility, . . . **Discussion:** what about your research centers?

Thank you for your attention

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