Towards Reproducible Research

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Overview

1. Introduction

Introduction: some definitions[1]

Repeatability and Reproducibility

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

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

→ **Reproducibility**: 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/x2lcg6a).

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Replicability

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 be equivalent if the same input data is provided.

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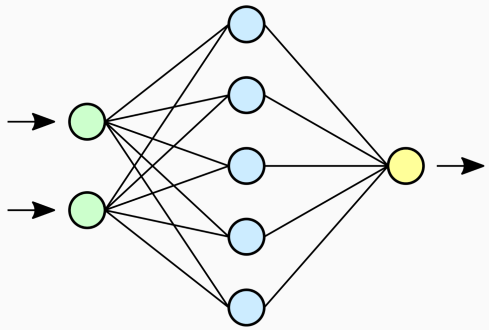
Definition: Repeatability Examples

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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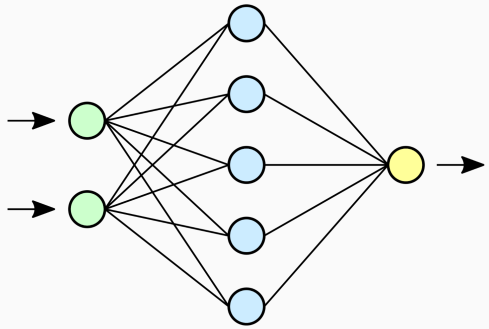

Not repeatable:

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

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.

$\Rightarrow$ 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.

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

Motivation: Example on Biomedical Research

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- Bayer HealthCare Germany confirmed: only 25% of cancer research is reproducible.
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Disciplines and RR

Different disciplines

- **Computational sciences**
- Biomedical, biology
- Social sciences
- ...

Each of them with their own requirements and protocols.

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- Computational sciences: no excuse!

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How can we perform RR with them?

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Statistical methods to decide if results are equivalent. I.e. hypotesis testing.

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Several reasons in general:

- Some researchers don't want to make public working code
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  - quality software takes more time to produce: testing, documentation, objective quality metrics, ...
- Results of a method do not generalize
- ... (For the discussion later!)

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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.ouvrirlascience.fr/second-national-plan-for-open-scienc
- "Path three: opening up and promoting source code produced by research"
- Not directly on reproducible research, but certainly fosters it
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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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2.2 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
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- **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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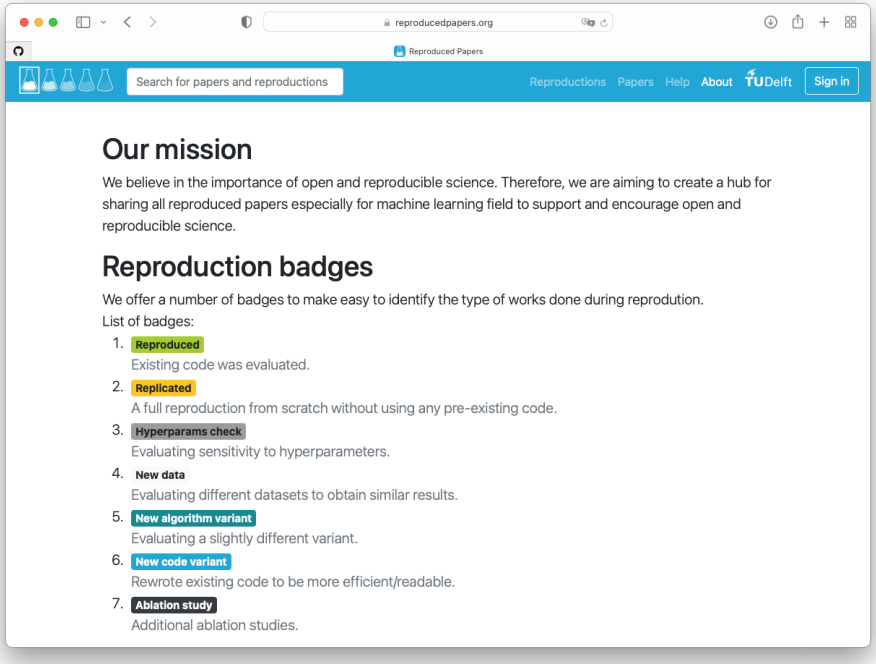

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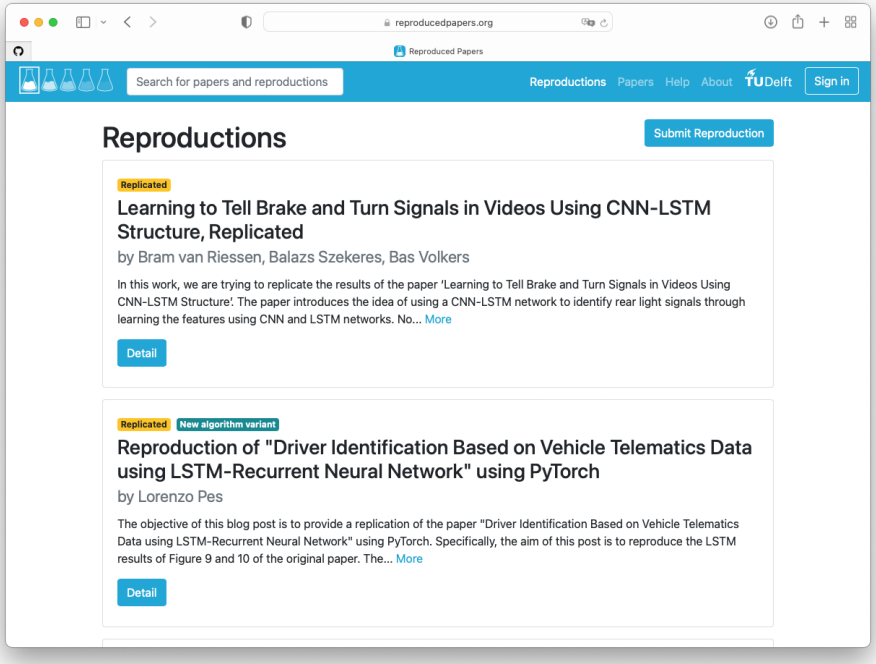

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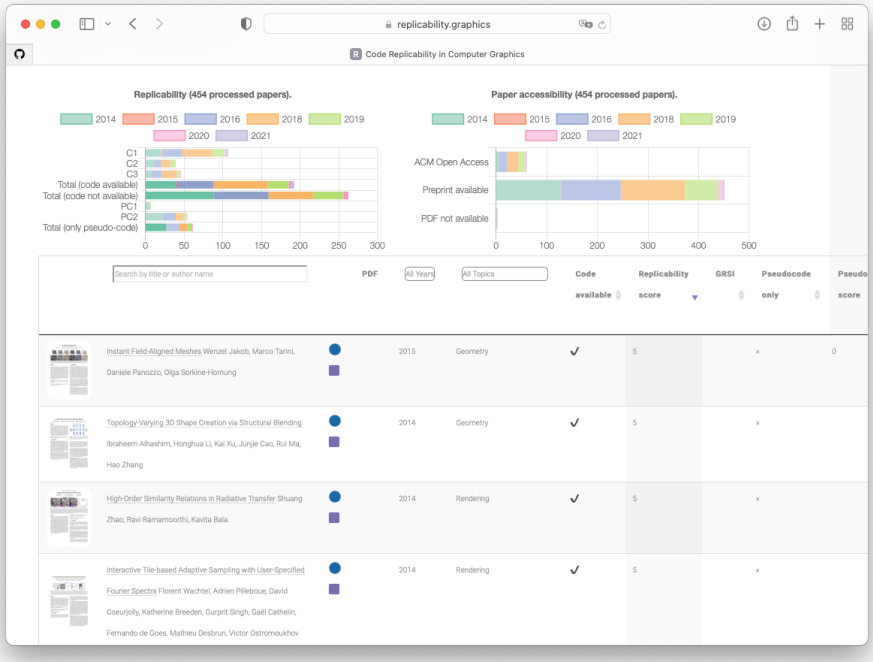

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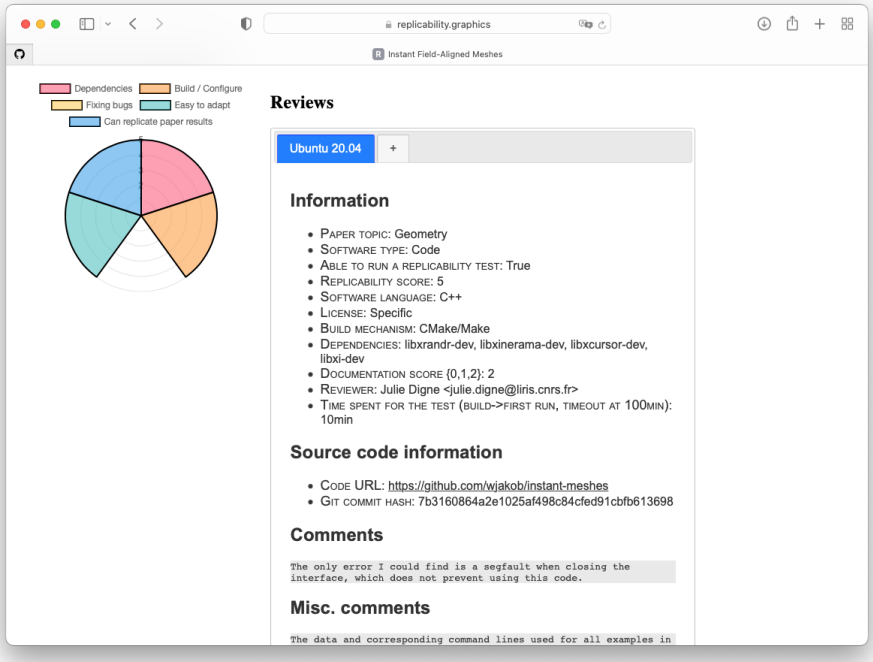

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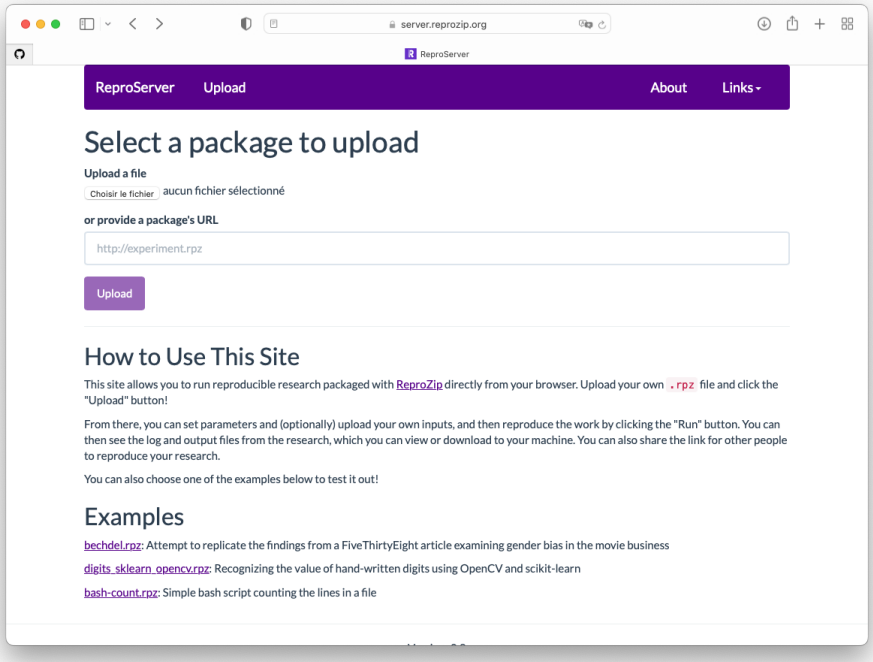

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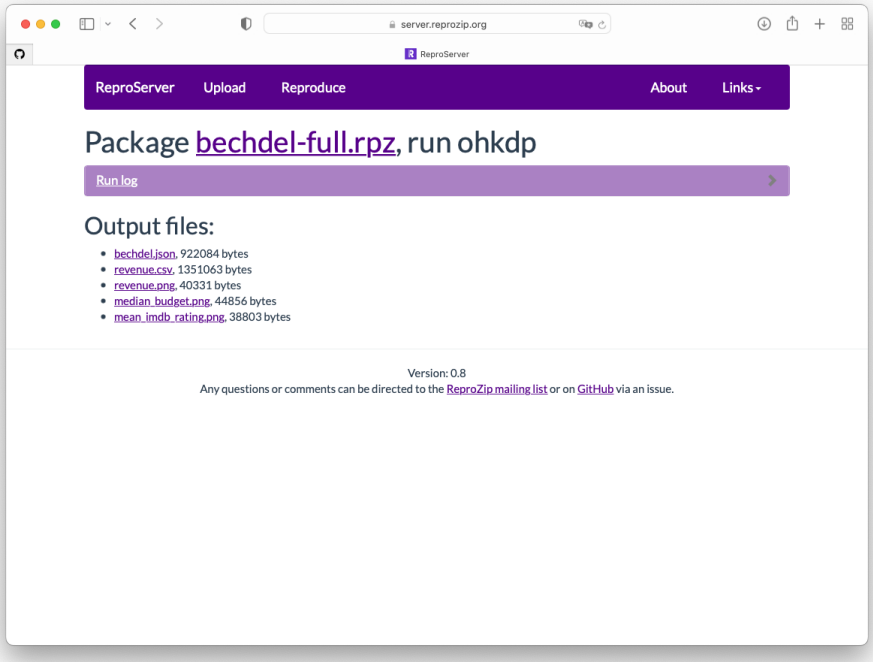
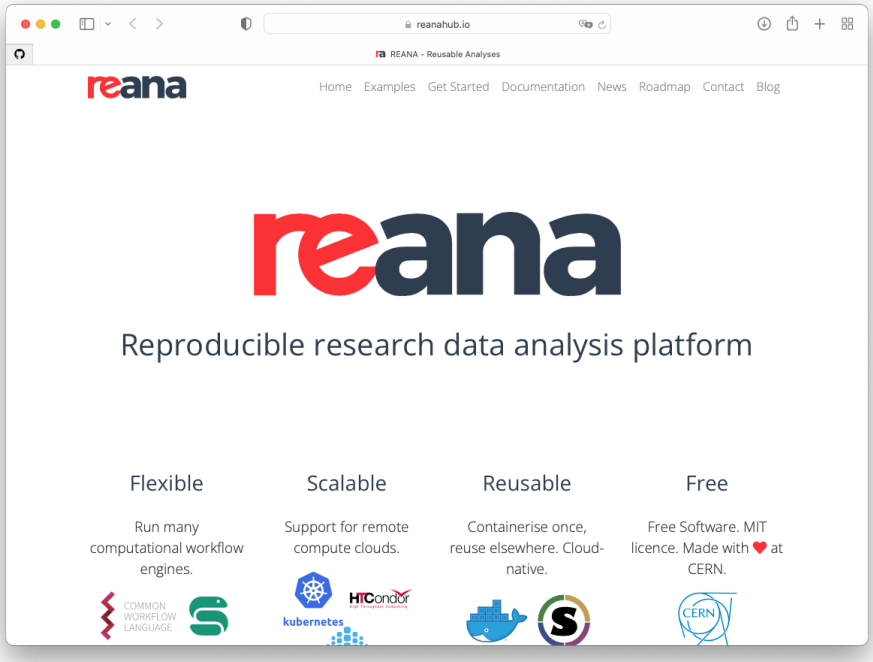


New Reproducible Research Platform (4)

Platform REANA : https://reanahub.io [Online execution platforms]

- Reproducible research data analysis platform.



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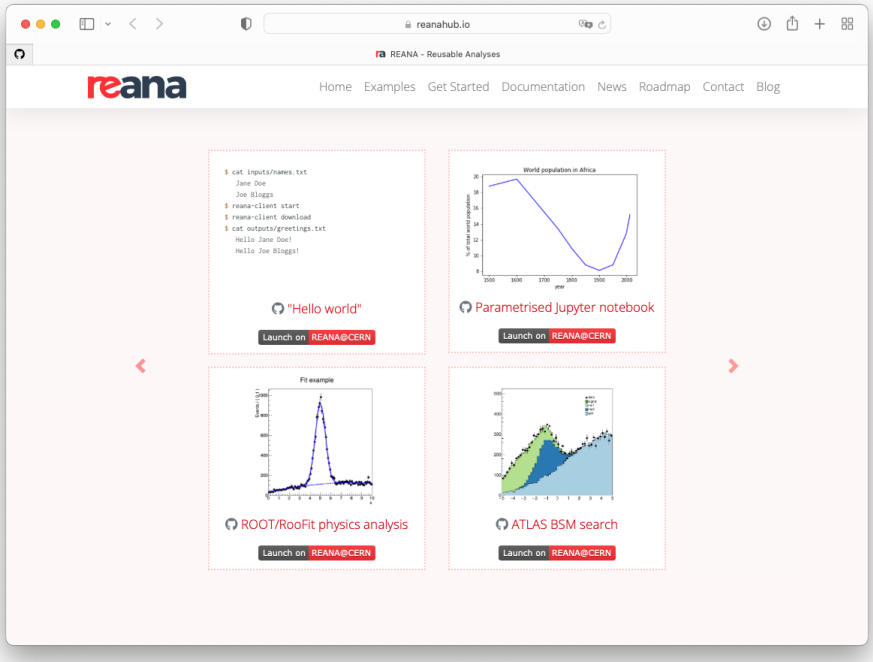

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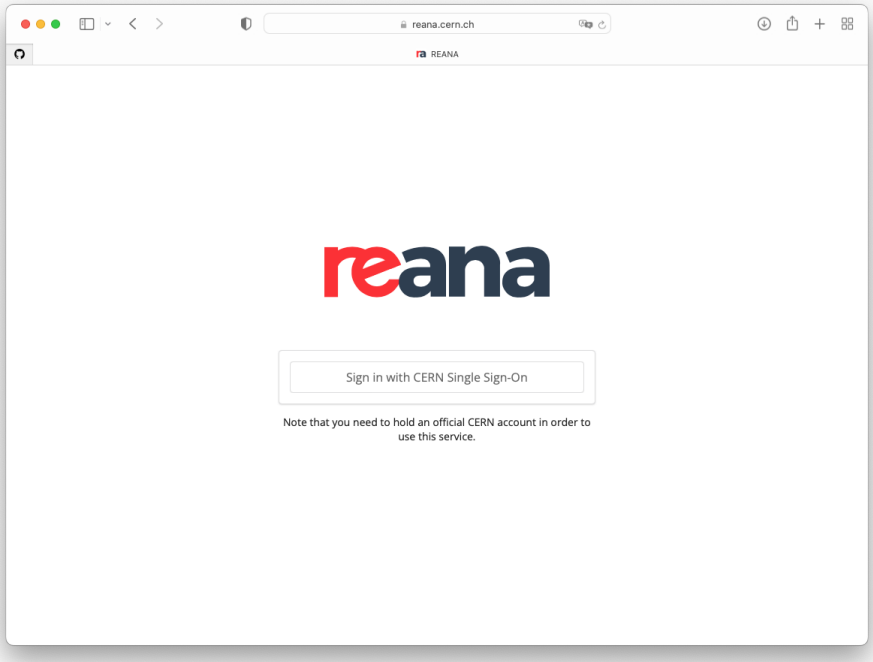

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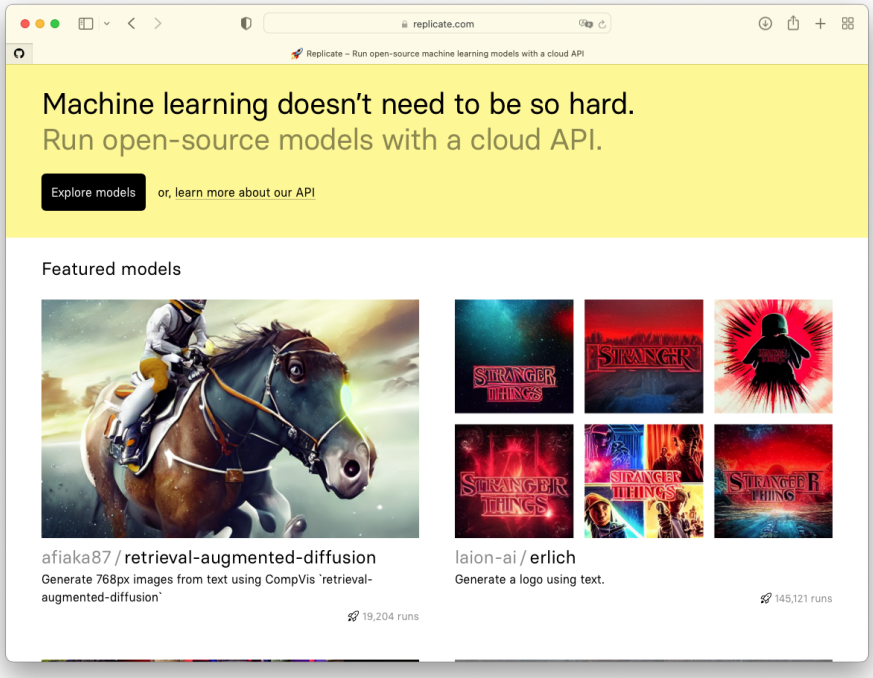

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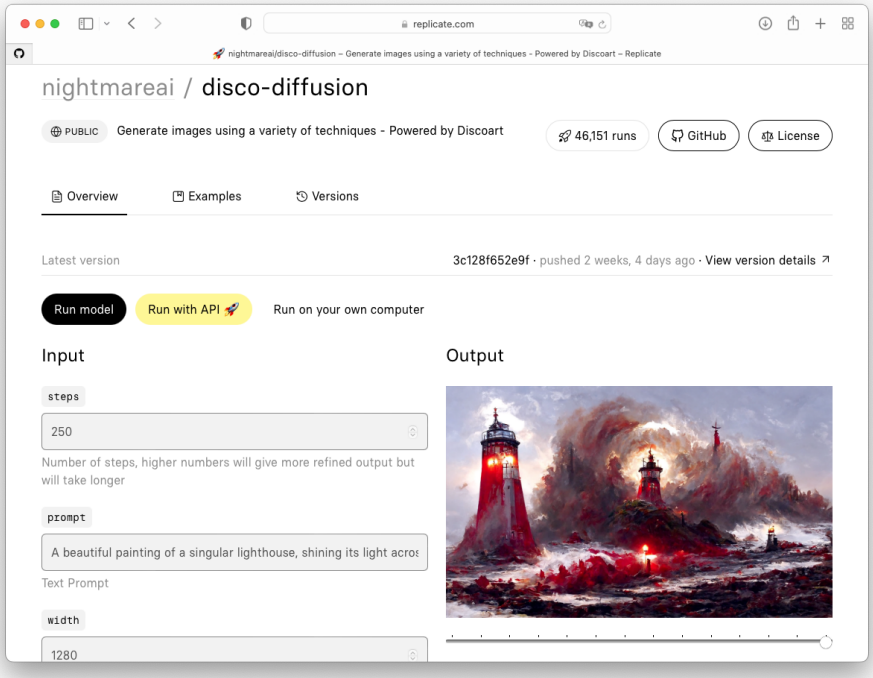

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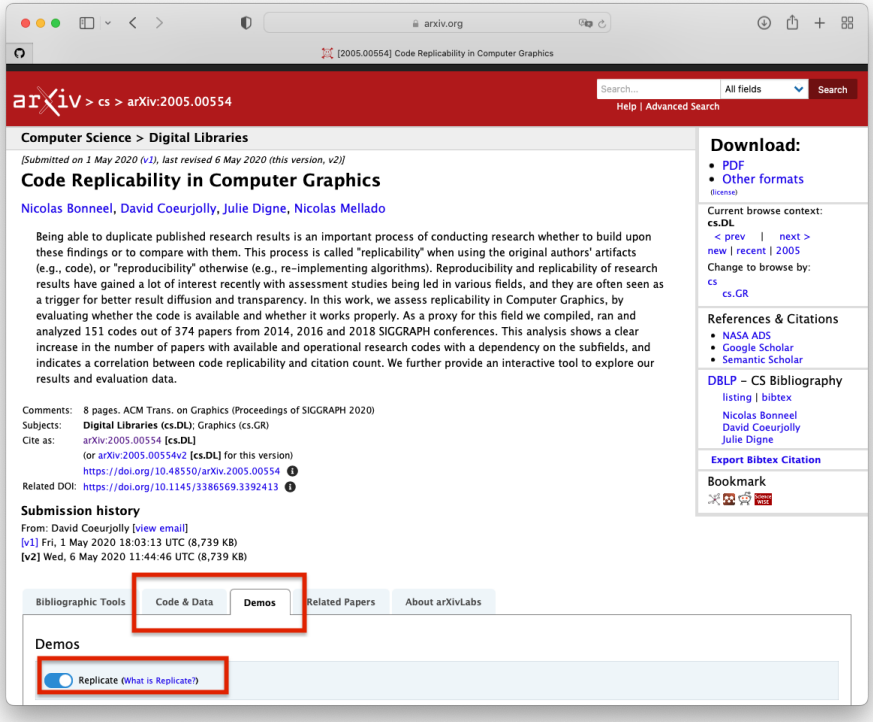

2.2 Library Development for RR

Libraries and contribution to RR

- Way to diffuse and reuse research methods
- Documented and referenced algorithms
- 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. **Discussion**: docker containers, replicability, reproducibility, maintainability.

2.2 Library Development for RR: examples (1)

Example of library of vision/image/geometry domains

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Long time efforts

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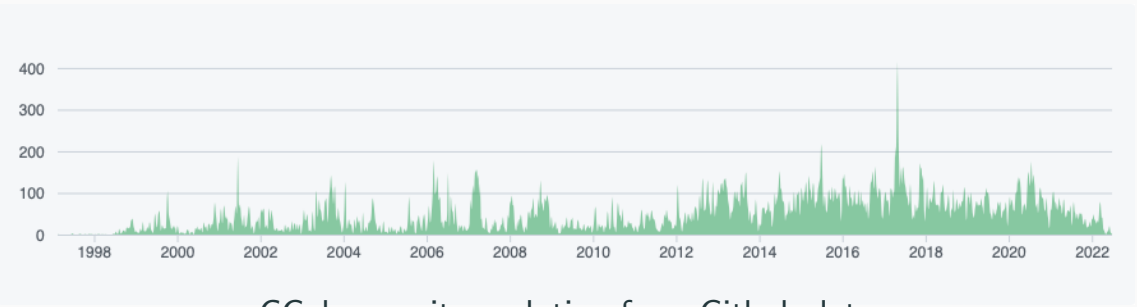

CGal commits evolution from Github data

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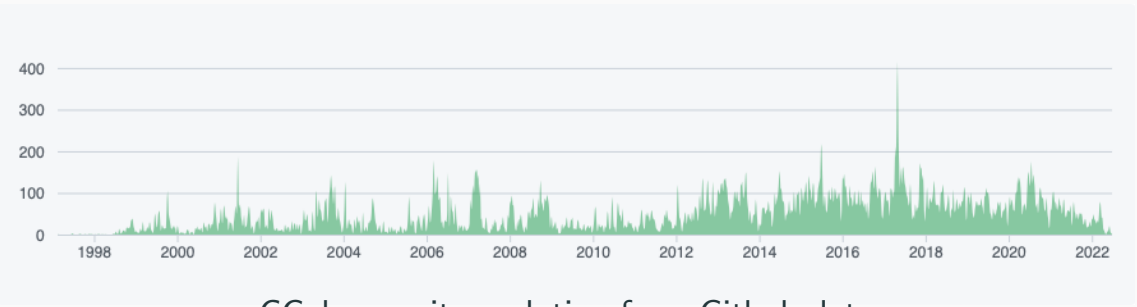
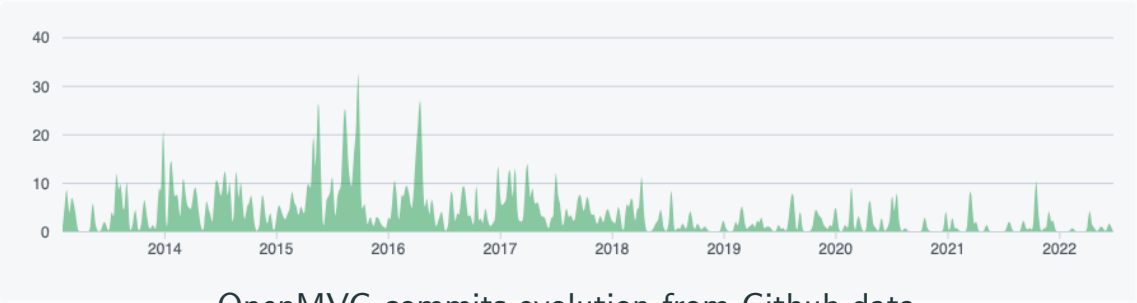


CGal commits evolution from Github data



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2.2 Library Development for RR: examples (2)

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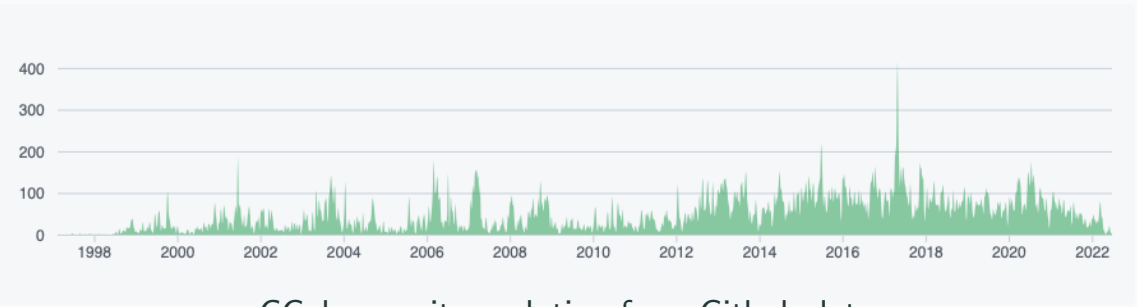

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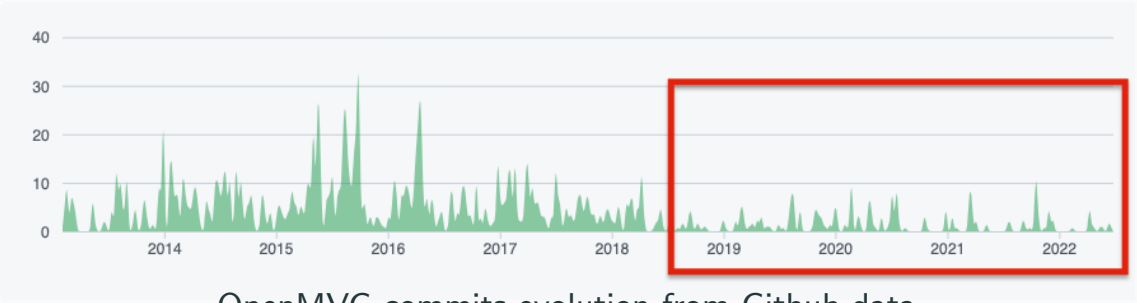

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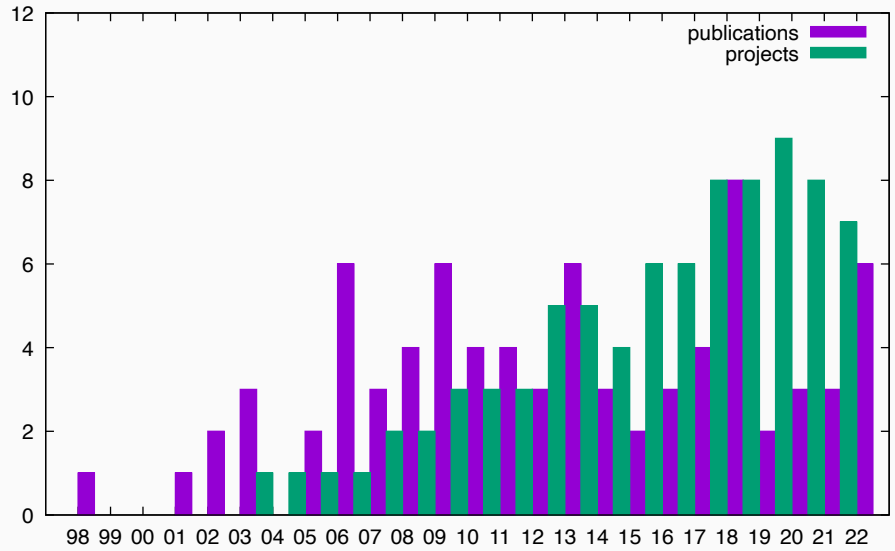
Example of impact measure

- 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

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

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$\Rightarrow$ 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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- Both the article (PDF) and the source 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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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.
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- 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 $\rightarrow$ same outputs)
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Difficulty

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

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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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- It has a **larger impact**, but it requires a **larger effort** too
- 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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