Research Data Management: A Perspective from the CRC 1194

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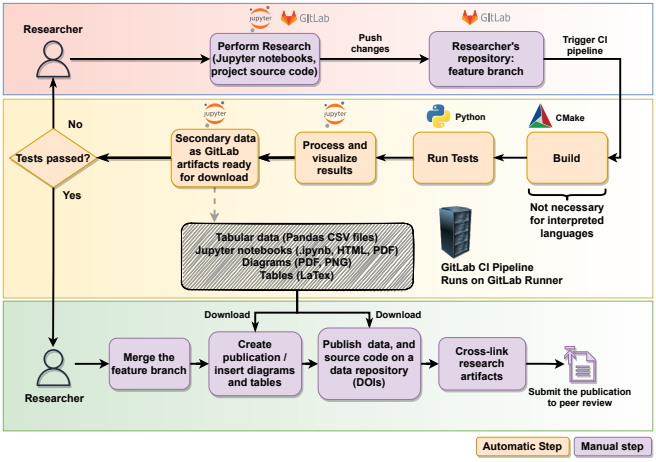

Two-phase flow simulation methods (B01, B02, Z-INF)

Validation, verification, and cooperations within the CRC1194

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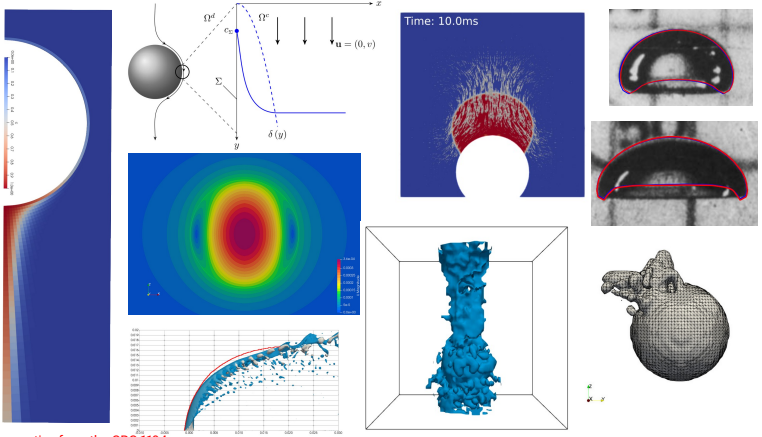

Collaborations between simulative and experimental projects

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Numerical simulation methods require thorough testing:

- Verification against exact solutions.
- Validation with respect to experiments.
- Serial and parallel computational efficiency: statistical performance experiments.

Experiments are adjusted using feedback based on numerical methods' results.

Collaborations within a CRC require data exchange

- Standardized, simple, interoperable secondary data/metadata format.
- Findable Accessible Interoperable and Re-usable (**FAIR**) Research.

FAIR research (data manegement) in a CRC

Boundary and initial conditions

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- Dedicated resources for handling research data are not available on project-level.
- Research data management concepts live or die with PhD students.
  - Cooperative publications are paramount in a CRC: cooperation overhead.
  - Research data management is checked increasingly critically.
  - Ph.D. candidates just want to graduate: anonymous poll showed 90% target industry positions.
  - Research data management causes some workload overhead.
  - **KISS: practical effective solutions, with very low overhead.**
  - **Research data publication as a Ph.D. defense requirement?**
- Ph.D. students rotate every funding period
  - Little or no overlap between successors and predecessors.
  - **Data processing pipeline automation and documentation.**

Research Data Management Concept of the CRC1194

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1. Use version control ("git").
   - Pays off when investigating / switching between different research ideas.
2. Automate and document (script) data-processing steps.
   - Pays off after several executions.
3. Implement case studies using literal programming (Jupyter Notebooks).
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4. Organize case studies to easily retrieve parameter-specific information.
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5. Focus first on secondary data, and use a simple data/metadata format.
   - Low hanging fruit, small data sizes.
6. Use milestones to cross-link digital research artifacts on data/publication repositories.
   - Satisfies the DFG requirement, takes half an hour.
7. Use Continuous Integration for automating research workflows.
   - Pays off during peer-review.

Version control

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- Management of versions of (usually) text data, like publications and scientific codes.
- Nowadays version control is **essential** for scientific codes of all shapes and sizes.
- Version control can be adapted to needs and constraints of the CRC[1].

[1] Maric, Tomislav, Lehr, Jan-Patrick, Papagiannidis, Ioannis, Lambie, Benjamin, Bothe, Dieter, & Bischof, Christian. (2021, April). A Workflow for Increasing the Quality of Scientific Software (Version 1.0). Zenodo. http://doi.org/10.5281/zenodo.4668439

Git version control system (VCS)

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- Use Overleaf for papers, Git for everything else.

Version control "enforces" modularity

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Git conflicts

- A file is changed differently on two branches and a merge is needed.
- Two team members edit the same file at once.

Modularity reduces conflicts and speeds up teamwork

- Separate implementation into separate version-controlled files.

Version control and Clean Code

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- University research teams are small (1 - few members).
- ▸ Separation of Concerns (SC) and ▸ Single Responsibility Principle (SRP) significantly simplify the branching model.
- **Separation of Concerns**: code is organized in non-overlapping layers and sections.
- **Single Responsibility**: functions or classes perform single clear tasks.
- SC and SRP can be applied to any software.
- Dogmatism should be avoided: single responsibility vs less responsibilities.

Integrating different versions (features, functionalities)

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Maintainers coordinate the integration.

- Keep the branching model (version structure) as simple as possible.
- Main and development branches are protected and managed by Maintainers.
- Maintainers are responsible for git tags and cleanup:
  - **Main**: integrations from accepted publications and development branch.
  - **Development**: integration of automatically-tested improvements.
  - **Feature**: reduce git-conflicts by separating responsibilities and concerns.

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Test Driven Development: Define Research Test Results First

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Test-Driven Development[2] for CSE

1. Do:
2. Define final test results you want to publish.
3. Define the evaluation of the test results.
4. Program top-down, i.e. write calls to non-existing functions.
5. Don't unit-test, yet! Only if a top-level test fails, dig deeper.
6. Implement a fix to a failing test.
7. While (tests fail)

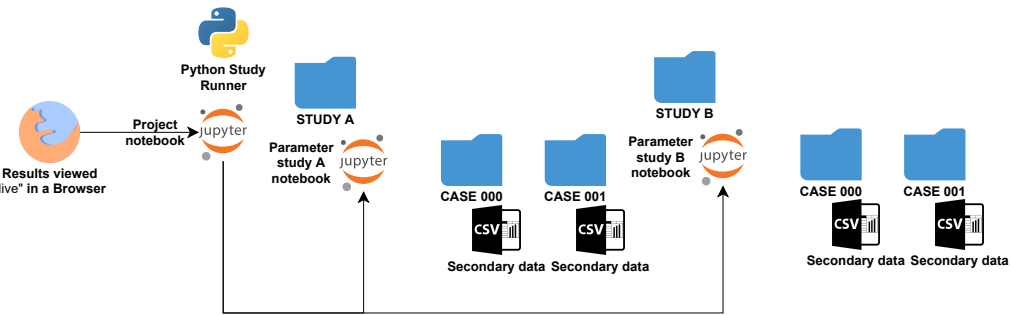
[2] Freeman, Steve, and Nat Pryce. Growing object-oriented software, guided by tests. Pearson Education, 2009.

Jupyter notebooks[3]

- **Documentation**: geometry, initial and boundary conditions, error norms, comparison data.
- **Processing**: verification errors (conservation, convergence, stability), validation errors.
- **Result analysis**: very straightforward, interactive, remote, directly-usable in publications!

[3] https://jupyter.org/

Case Parameterization



- Don't store metadata in folder names.
- Generate locally-unique case ID's, each Case ID mapping to a Parameter Vector.
- Store the mapping (Case ID $\rightarrow$ Parameter Vector) in a simple format (CSV).

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Importance of Secondary Data

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Secondary Data (tables, diagrams)

- Decide if a paper will be accepted or rejected.
- Are the basis for communication in CRC's cooperations.
- Are the basis for comparison of research results from literature.
- Are very small and easily manageable.

Standardizing Secondary Data

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- We compare data from studies involving parameters.
  - Physical parameters.
  - Method parameters.
- Study parameters are metadata, results are data.
- We need to easily compare results between different parameter sets.
- We need to easily investigate correlations in the parameter space.
- Parameters are often varied in a structured way, naturally leading to Hierarchical Data Format.

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- The Hierarchical Data Format[4] is a data format specification.
- HDF5 encodes a hierarchy of data items with their metadata and supports grouping data.
- HDF5 is an interoperable and open standard.
- HDF5 is implemented for scalable parallel Input / Output.
- HDF5 implementations exist in many programming languages.

[4] Collette, Andrew. Python and HDF5: unlocking scientific data. " O'Reilly Media, Inc.", 2013.

Standardizing Secondary Data

Hierarchical Data Format: HDF5 II

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```
File: example.h5
+-- Attributes
|   +-- experiment_name: 'Sample Experiment'
|   +-- experiment_date: '2024-07-01'
|   \-- description: 'Sample description.'
+-- group1
|   +-- Attributes
|   |   \-- description: 'This group contains data from sensor 1'
|   \-- data1
|       +-- Attributes
|       |   +-- units: 'meters'
|       |   +-- description: 'Distance measurements from sensor 1'
|       |   +-- physical_quantity: 'distance'
|       |   +-- calibration_date: '2024-06-30'
|       |   \-- calibration_coefficient: 1.01
|       \-- Data: [0.123, 0.456, 0.789, ...]
```

Standardizing Secondary Data

Hierarchical Data Format: HDF5 III

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```
\-- group2
    +-- Attributes
    |   \-- description: 'This group contains data from sensor 2'
    \-- data2
        +-- Attributes
        |   +-- units: 'meters'
        |   +-- description: 'Distance measurements from sensor 2'
        |   +-- physical_quantity: 'distance'
        |   +-- calibration_date: '2024-06-29'
        |   \-- calibration_coefficient: 0.98
        \-- Data: [0.234, 0.567, 0.891, ...]
```

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Now let's try to get data from sensor with calibration coefficient $\in [0.9, 1]$

```
with h5py.File('example.h5', 'r') as f:
    def check_group(group):
        for key, item in group.items():
            if isinstance(item, h5py.Group):
                # Recursively check sub-groups
                check_group(item)
            elif isinstance(item, h5py.Dataset):
                # Check if the dataset has the attribute
                if 'calibration_coefficient' in item.attrs:
                    coeff = item.attrs['calibration_coefficient']
                    if min_coeff <= coeff <= max_coeff:
                        print(f"Dataset: {item.name},
                        Calibration Coefficient: {coeff}")
```

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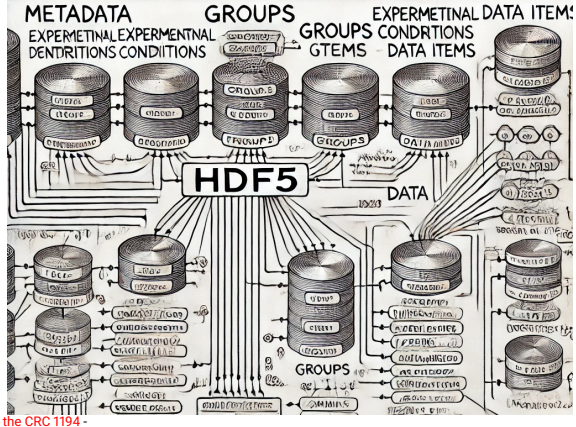
This is how ChatGPT and I together see HDF5 for secondary data :)



A Simple Format for Secondary Data and Metadata I

It's just a simple table.

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- **We leverage the small size of secondary data**[5]
- We store metadata and data as columns in a table.
- We store the table as CSV and use Python Pandas to work with it.
  - Yes, you can also use Excell.
- **We duplicate metadata**, we don't care, because
  - We get a 100% interoperable dataset.
  - This trivializes data analysis, exchange, and comparison.

[5] Marić, Tomislav, et al. "A pragmatic workflow for research software engineering in computational science." arXiv preprint arXiv:2310.00960 (2023).

A Simple Format for Secondary Data and Metadata II

It's just a simple table.

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Blue are metadata, red are (secondary) data.

PARAM_HIDDEN_LAYERS	PARAM_OPTIMIZER_STEP	PARAM_MAX_ITERATIONS	PARAM_EPOCH	TRAINING_MSE	
10,10,10,10	0.0001	3000	1	1.091560	
10,10,10,10	0.0001	3000	2	1.082970	
10,10,10,10	0.0001	3000	3	1.077200	
10,10,10,10	0.0001	3000	4	1.072650	
...	...	...	...	...	...
10,10,10,10	0.001	3000	1	0.992354	
10,10,10,10	0.001	3000	2	0.991959	
10,10,10,10	0.001	3000	3	0.995102	
10,10,10,10	0.001	3000	4	0.996143	
...	...	...	...	...	...

A Simple Format for Secondary Data and Metadata III

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Let's do some basic research using this secondary data format.

- Sub-sample using metadata intervals

```
data = study[(study['calibration_parameter'] >= 0.9) and
             (study['calibration_parameter'] <= 1.1)]
```

- Analyzing correlations of data w.r.t. metadata is equally easy.
- Comparing results from two studies

```
value_columns = [col for col in df1.columns
                 if not col.startswith('PARAM_')]
difference_df = study1[value_columns].copy() -
                study2[value_columns].copy()
```

- Pandas is one line of code away from Numpy, i.e. from Machine Learning.
- We haven't used it on primary data, but first examples seem to work.
  - We only duplicate metadata!

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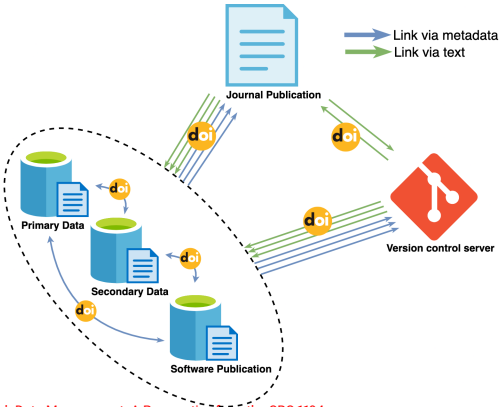
Cross-linking data, source code and reports/publications I



Cross-linking milestones

- A pre-print is ready for publication.
- A publication is revised and ready for re-submission.
- A publication has been accepted for publication.
- A PhD thesis is ready for submission.
- A method has found not to work.

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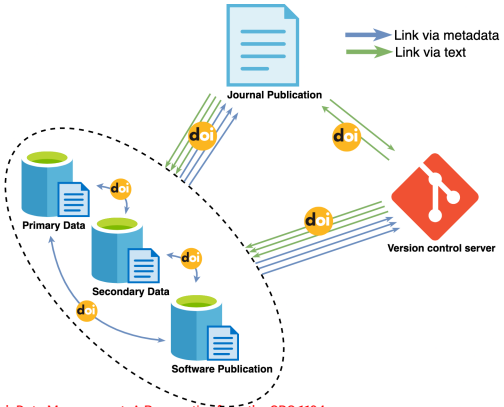
Cross-linking data, source code and reports/publications II



- Save Overleaf label and / or "tag" the manuscript version.
- Upload data and software to a data repository.
  - Zenodo.org is not indexed by Google (Scholar).
  - While data citations don't help you, indexed data links to papers!
- Cite data and software in the preprint.
- Upload pre-print, obtain it's DOI.
- Add pre-print DOI to data and software metadata on the data repository.

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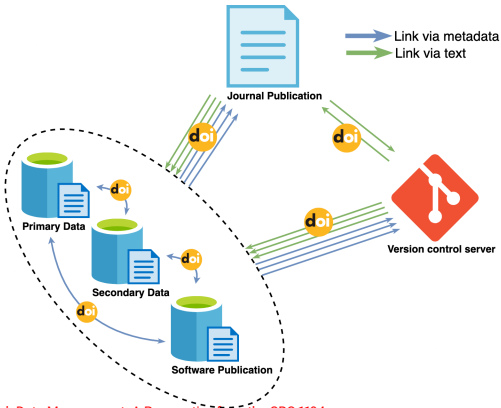

- First time it takes an afternoon, second time it takes 10-15 minutes.
- Data and software increases citation count and visibility (subjective observation).
- How long does it take to get results, generate software, data, and write the preprint?
- How much tax funds is behind a single DFG-funded publication?
- We should strive to ensure FAIRness of our research as scientists.

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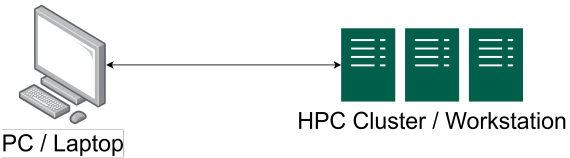
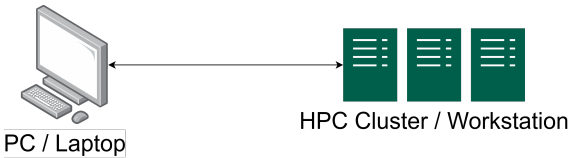


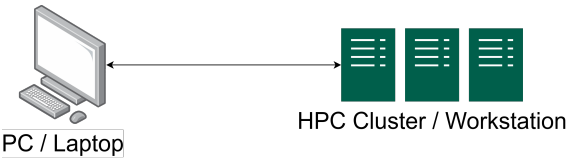
while Results are unsatisfactory **do**
    Implement some data-processing code.
    (Compile the code.)
    for All studies **do**
        Run the study.
        Analyze results.
    end for
    Compare old and new results.
end while



Issues...

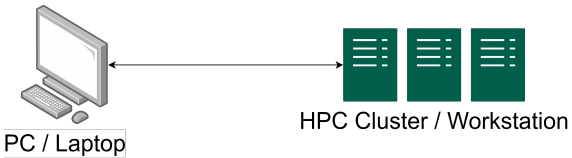
- Starting studies takes time.
- Analyzing results takes time.
- Often the results are not checked "live" as the study runs - **waste of research time and CPUh**.
- **Only the researcher knows the details** behind the initialization, running and post-processing scripts - **when this person leaves, the reproducibility is gone.**
- A researcher may forget to run a study and believe all tests have passed.

Continuous Integration of Scientific Software III



while Results are unsatisfactory **do**
    Implement some data-processing code.
    (Compile the code.)
    for All studies **do**
        Run the study. ▷ Manual.
        Analyze data. ▷ Manual.
    end for
    Examine results. ▷ Manual.
end while

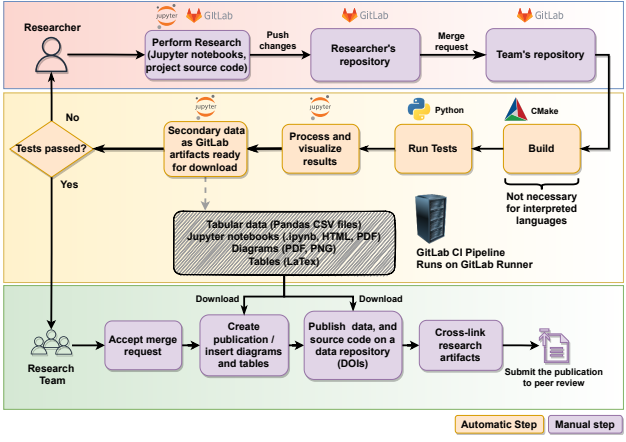
Continuous Integration of Scientific Software III



while Results are unsatisfactory **do**
    Work on algorithms.
    (Compile the code.)
    Run the studies (jobs). ▷ Automatic.
    Run data analysis (jobs). ▷ Automatic.
    Examine results. ▷ Manual.
end while

(Continuous) Integration of scientific software IV

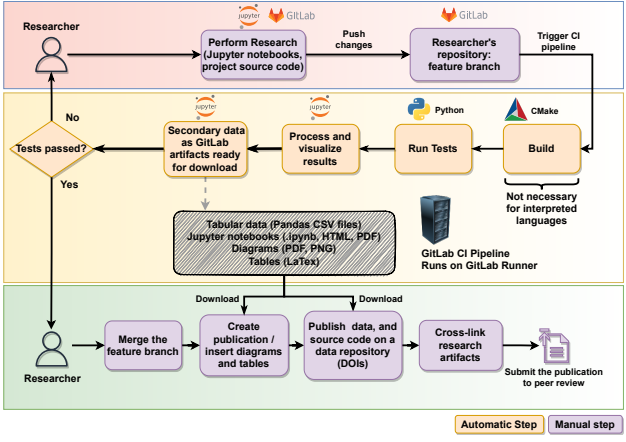
Schematic diagram for the team workflow



Working in a team.

(Continuous) Integration of scientific software V

Schematic diagram for the individual workflow



Working alone.

(Continuous) Integration of scientific software VI

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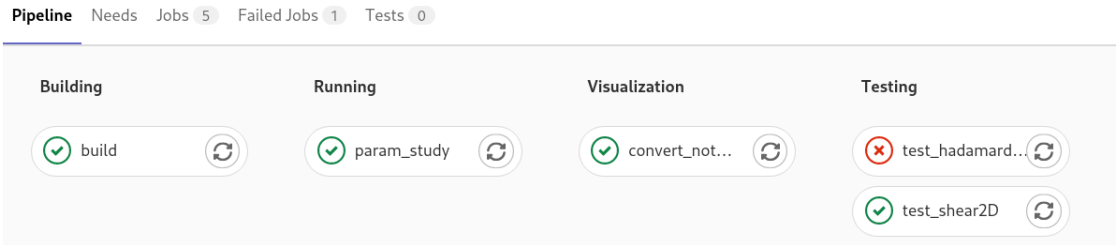
An example CI pipeline you can view in your favorite browser



(Continuous) Integration of scientific software VII

CI in a nutshell II

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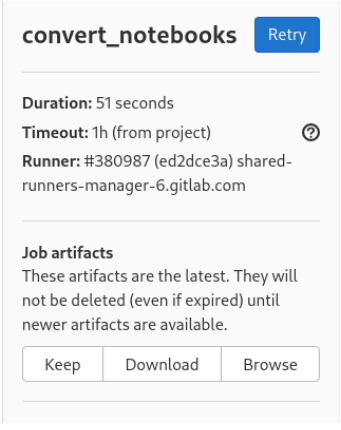
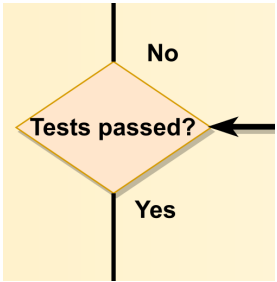


- Files created within a CI job are gone when the job ends.
- GitLab uses **job artifacts** to pass on data from one job to the next.
- **Job artifacts can only be files stored in project's sub-folders.**
- Libraries and applications are passed to other jobs as artifacts.
- **Artifacts can be downloaded on the GitLab project website.**

(Continuous Integration with result visualization) I

Test evaluation I

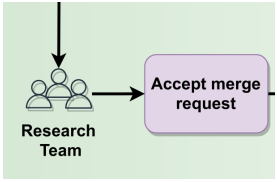


Straightforward for easily quantifiable errors

- **Examples:** volume conservation, order of convergence, total wall clock time, weak scaling, ...
- **Python scripts test secondary data** agglomerated by Jupyter notebooks from simulation results.

(Continuous Integration with result visualization) II

Test evaluation II



Difficult for errors that cannot be quantified easily

- **Examples:**
  - Is is the difference between simulation and experiment data $\leq 4\%$?
  - How to quantify the difference for complex signals?
- **Option 1: Researchers evaluate the test results even if all CI jobs pass.**
  - A simple and efficient solution 🎓.
- **Option 2: Use statistics to quantify the difference.**

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Interaction between Transport and Wetting Processes

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