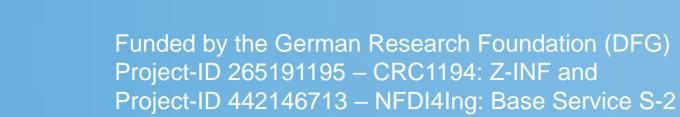
A Research Software Engineering Workflow for

Computational Science and Engineering

PASC23, 2023-06-26, Davos, Switzerland

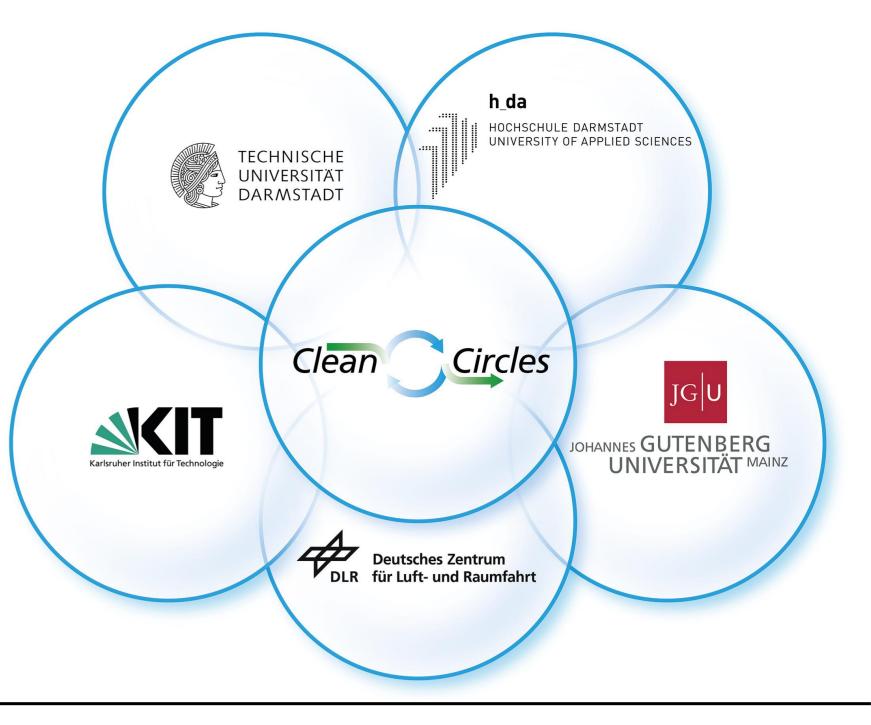


Schwarzmeier Maric





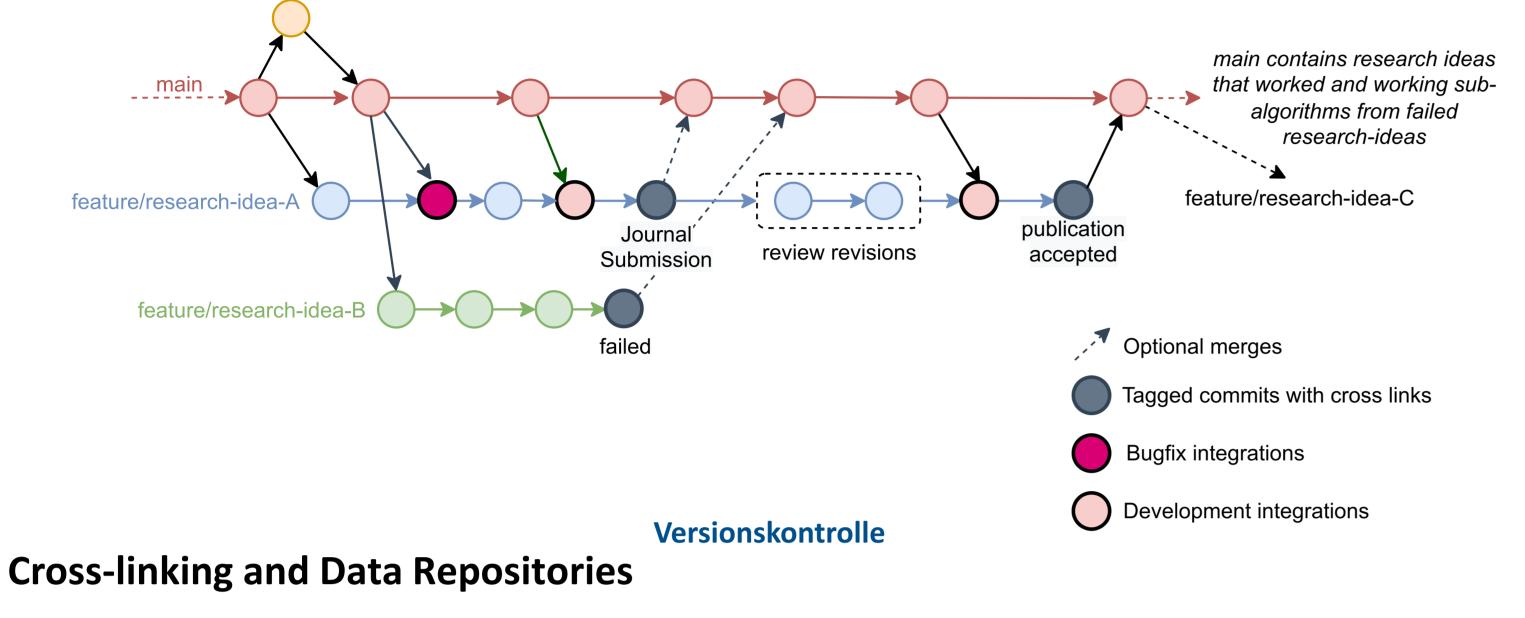
Wechselseitige Beeinflussung von Transport und Benetzungsvorgängen



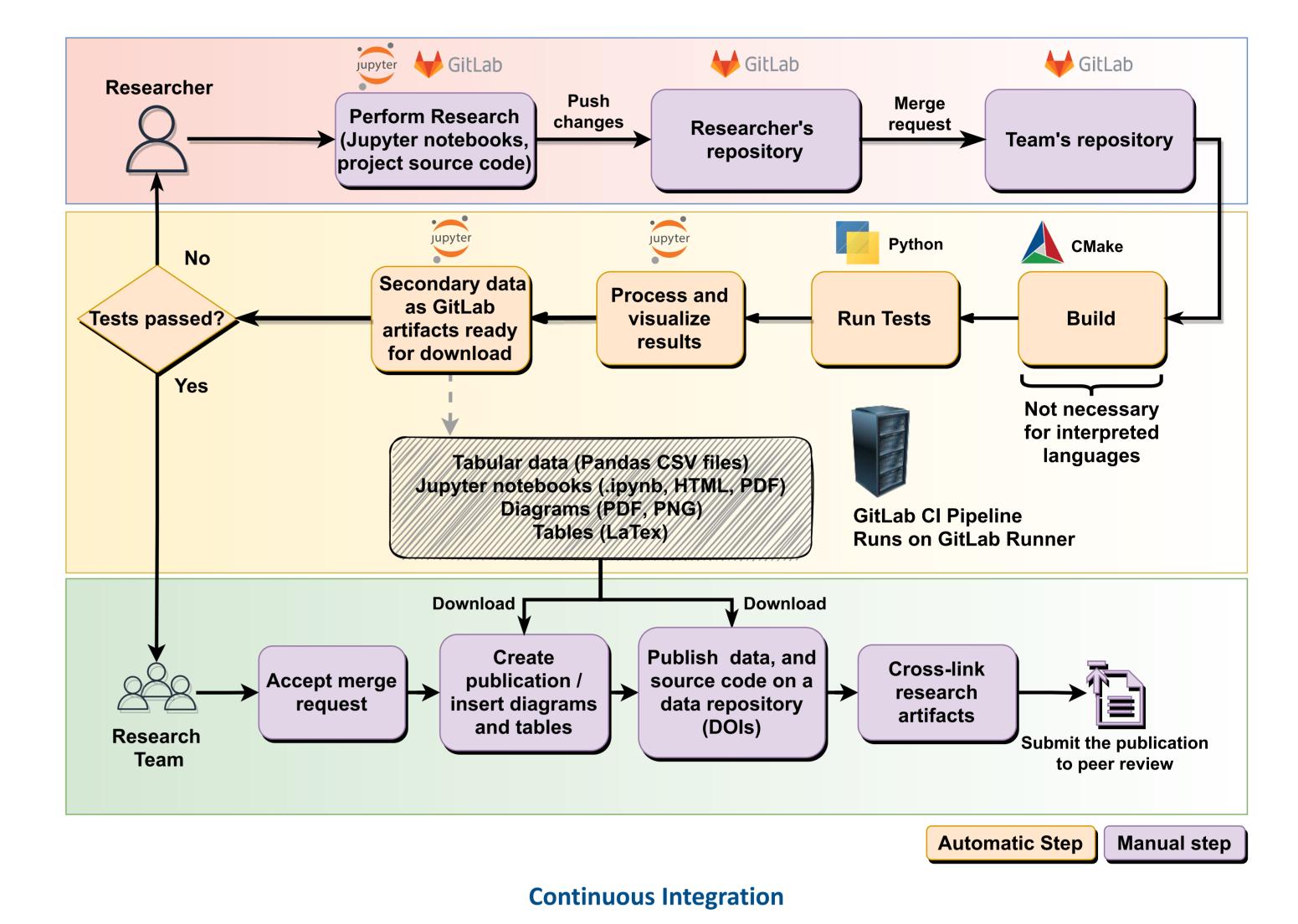
Open Data Concept enabling Traceability

Version Control and Branching Model

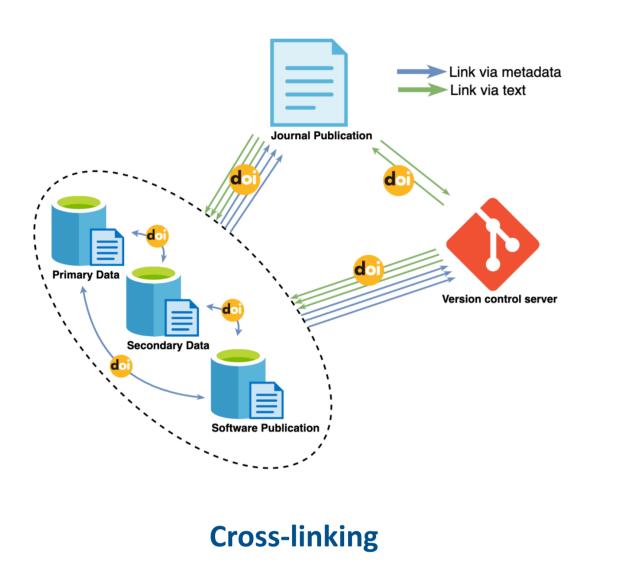
- Tracking of changes is possible \rightarrow Findability
- Enables continuous development of a single main version \rightarrow Sustainability



Continuous Integration (CI)



- Linking of research data, articles and software
- Retrievable, unique and persistent

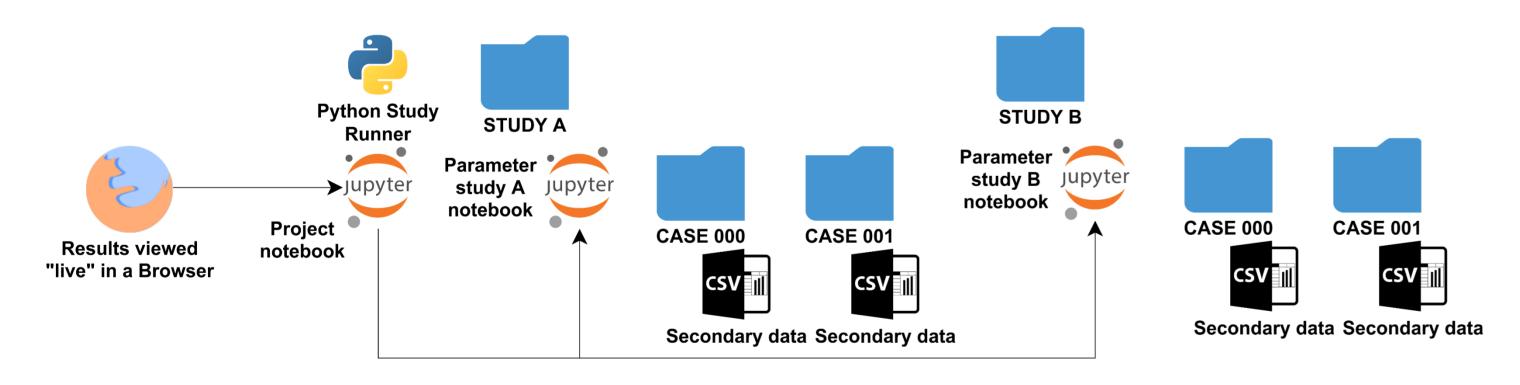


- Integration successfull only, if there are existing tests.
 - Reproducibility
- **CMake**: cross-platform build system
 - > Simplified dependencies between software projects

 \rightarrow Sustainability

- Jupyter Notebooks:
 - > **Detailed test documentation** with integrated results/comparison data
- **GitLab CI artifacts**: download of the test results

Folder Structure ensures Clarity and Readability



Parameter study structure

- Folder structure ensures clarity and machine readability:
 - One top level folder per parameter study and
 - One low level folder per case
- Parameter study notebook describes parameter study and displays secondary data

Knowledge Base

We run a Knowledge Base in Collaboration with NFDI4Ing

> home - Knowledge Base · × +		
← → ♂ @ O A https://knowledge-base.nfdi4ing	de 50% 🖈	
NFDi4ing		
Q. Bearch.	GETTING STARTED	
🖨 Home	This knowledge base is based on A workflow for increasing the quality of scientific software 🏝 (Maric Lehr et al. to be published) a paper that originated from the work at the SEB 1194 at TU	

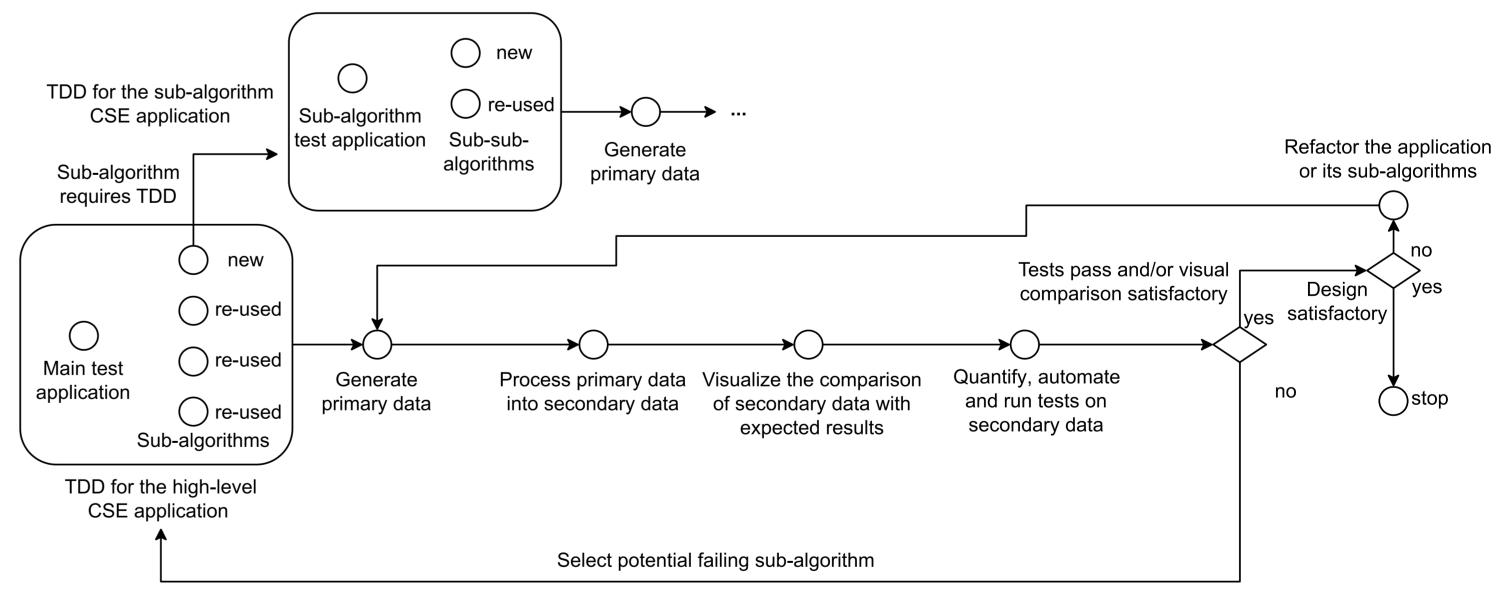
Opening a Merge Request on GitLab
If you already have a <u>feature-branch</u> that you want to <u>merge</u> , in collaborative projects it is best to open a <u>Merge Request (MR)</u> on <u>Mab</u> , where all the collaborators can revise and discuss the new feature A branch is a development line.
Another great possibility to open a MR is from an existing 'Issue', where a branch will be created a

- Python test suite classifies the test results for GitLab CI
- **CI documents workflow** that is guaranteed to be up to date

Challenges

- **Docker (/Apptainer) images** \rightarrow <u>Reproducibility</u> of primary data
- **Convergence studies might require HPC resources**
 - Legal, security, funding, portability, ... concerns.
 - Reduction of (convergence) testing?

Top-down Test-Driven Development



Testing approach for complex, open source and modular software (like OpenFOAM)

Darmstadt. For this paper please see our section in literature. We presented this knowledge base at the FOSDEM'22 HPC devroom. Go directly to the video recording or move to our notification.
The articles herein are equipped with tags to help find them as well as they are labeled with the chapters according to the sectioning of aforementioned paper, namely Version control, Build system, Cross-linking publication, software and datasets, Continuous Integration, Containerization, Test-driven development and code quality, Test quantification, visualization and evaluation on HPC-clusters and th category, whether the article belongs to a minimum or a full workflow.
It is recommended to read the paper carefully and to try to follow the Getting started in the guides-section.
Consultation hour
OTp
We are now offering consultation hours every wednesday at 10 AM (Berlin, CET/CEST). Simply click this link. In case you can not join, please contact Moritz Schwarzmeier .
Contributing
We are always happy about people helping us to build a better knowledge base. Please reach out to us.
Supported by
Funding
The authors would like to thank the Federal Government and the Heads of Government of the Länder, as well as the Joint Science Conference (GWR), for their funding and support within the framework of t NFDI4Ing consortium and the SFB 1194. Funded by the German Research Foundation (DFG) - project numbers 442146713 and 265191195.
Website creation
NFDi4ing
NFDI4ing

https://knowledge-base.nfdi4ing.de

- Topics: Version Control, Cl, Build Systems, Cross-linking, Container, TDD, Test evaluation Guidelines
- Guides with code examples
- Literature





We offer consultation hours every wednesday.

- Peer-reviewed
- Under constant revision
- Taxonomies (tags, chapters)
- Participants from
 - Software development
 - Engineering
 - Research data management

Test functionality, not implementation!

- Assume all sub-algorithms are running.
- Break down non-working algorithms into sub-algorithms.
- Refactor only the running algorithms.

Further Information

- **Knowledge Base:** https://knowledge-base.nfdi4ing.de
- **Preprint** about this Workflow:
 - A Research Software Engineering Workflow for Computational Science and Engineering;

Marić, Gläser, Lehr et al., 2022, https://doi.org/10.48550/arXiv.2208.07460

- **Slides with exercises** regarding this workflow:
 - "Continuous" Integration of Scientific Software (in Computational Science and Engineering);

Marić et al., 2021, https://zenodo.org/record/5522820.YnTOvnVByXI

This poster: https://doi.org/10.5281/zenodo.7930299