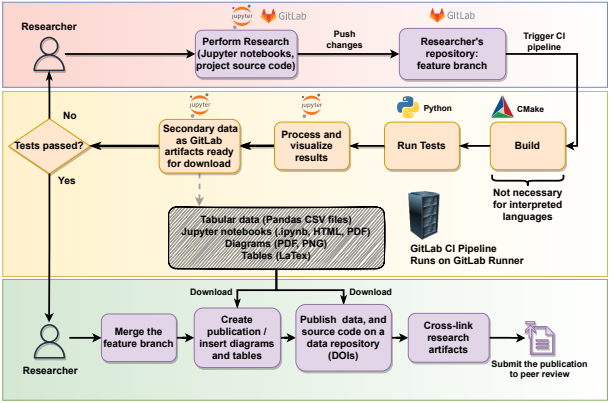
A Research Software Engineering Workflow for Computational Science and Engineering

SFB1194/Z-INF, Base Service S-2 *Research Software Development*

TECHNISCHE UNIVERSITÄT DARMSTADT



NFDi4Ing

Computational Science and Engineering software in university research groups

Boundary and initial conditions

TECHNISCHE UNIVERSITÄT DARMSTADT

- Publish or perish 🎓[1] prioritizes publications over scientific software.
- Dedicated resources for increasing software quality are usually not available.
- Ph.D. students rotate every 3-5 years, postdocs every 1-2 years.
  - Little or no overlap between successors and predecessors.
- Large-scale software design is not a mandatory part of the CSE curriculum.
  - Different CSE background: (Applied) Mathematics, Mechanical Engineering, Physics, Informatics.

[1] Symbol of a publish-or-perish simplification of the workflow :)

Computational Science and Engineering software in university research groups

The chaos scientific legacy code

TECHNISCHE UNIVERSITÄT DARMSTADT

Betty is a CSE researcher, working with a legacy research code.
Why is Betty so (rightfully) angry?

- Betty inherited a **research software that is only partially tested**.
- Betty inherited a **research software that isn't automatically tested**.
  - Betty changes one part of the code and gets her model running, only to see 10 other things fail, after days of manually running tests.
- Betty's software has **no documentation of the scientific workflow**.
  - Betty doesn't know how to use existing scripts to run simulations and analyze (reproduce) results.
- Betty's software has **disjoint (diverging) versions** - that she can't integrate.
- **Betty can't even find code versions used to generate results in the publications from her research group.**

Computational Science and Engineering software in university research groups

Continuous integration and cross-linking to the rescue

TECHNISCHE UNIVERSITÄT DARMSTADT

Automated testing (verification and validation), **version control**, and **cross-linking** reports, source code and research data increase Findability, Accessibility and Reproducibility (FAIR) and **speed up research.**

- **Continuous Integration (CI) = automatic testing + version control.**
- CSE research requires **scientific workflows**: initialize simulations, run parameter variations, agglomerate data, visualize, and check results.
- CI can be used to **automate and document scientific workflows**.
- CI ensures that the **integration of new changes does not break existing functionality**.
- Once the changes are integrated, the publication, the source code and the data are published on pre-print and data repositories and **cross-linked** using git tags and DOIs.

TECHNISCHE UNIVERSITÄT DARMSTADT

while Results are unsatisfactory **do**
    Work on algorithms.
    (Compile the code.)
    for All studies **do**
        Prepare the study.
        Run the study.
        Analyze results.
        Move results to a report.
    end for
    Compare old and new results.
end while

A Research Software Engineering Workflow

Collecting the components: Automation I

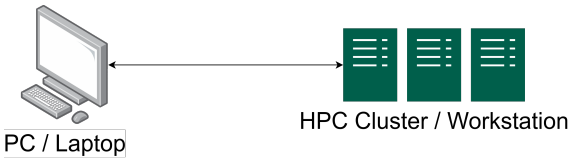
TECHNISCHE UNIVERSITÄT DARMSTADT

while Results are unsatisfactory **do**
    Work on algorithms.
    (Compile the code.)
    for All studies **do**
        Prepare the study.
        Run the study.
        Analyze results.
        Move results to a report.
    end for
    Compare old and new results.
end while

while Results are unsatisfactory **do**
    Work on algorithms.
    (Compile the code.)
    Run initialization scripts (jobs).
    Run simulation scripts (jobs).
    (Run postprocessing scripts (jobs)).
    Visualize results live in Jupyter notebooks.
end while

A Research Software Engineering Workflow

Collecting the components: Automation II

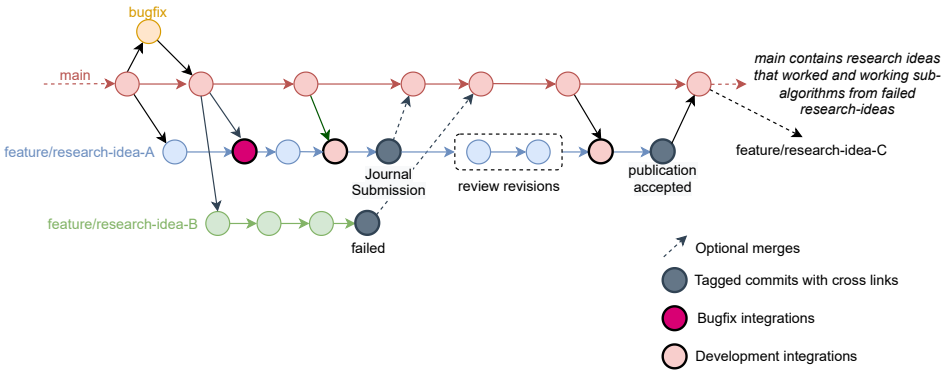


- **Manual testing takes a lot of time**.
- **Manual testing** of all previous tests **is prone to error** - even if V&V scripts do not require metadata.
- **Only the researcher knows the details** behind the initialization, running and post-processing scripts
- Relevant **V&V tests are automated using Continuous Integration (CI)**.
  - The remote repository starts the so-called **CI** test pipeline (a sequence of tests).
  - All tests are automatically run, processed and visualized.

A Research Software Engineering Workflow

Collecting the components: Version Control

TECHNISCHE UNIVERSITÄT DARMSTADT

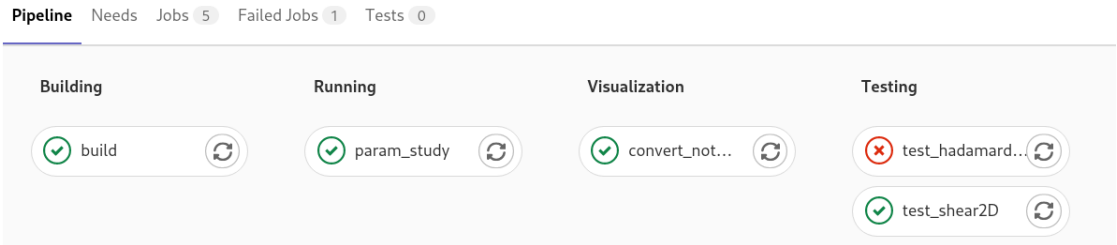


The branching model increases reproducibility.

TECHNISCHE UNIVERSITÄT DARMSTADT

- A **text (YAML) file** is added to a repository, that **specifies the tests** (jobs) in a CI pipeline.
- When the YAML file is pushed to an upstream git repository (GitLab), **GitLab creates a CI pipeline from the YAML file**.
- The CI pipeline needs a **machine for running tests - the GitLab runner**.
  - Shared runners on gitlab.com have limited capacity.
  - We can install and register our own GitLab runner.
- **A Docker image encapsulates the computing environment**.
  - **Virtualization/Containerisation** increases reproducibility and simplifies testing.
- The Docker image must be publicly accessible for it to be used by a shared runner.

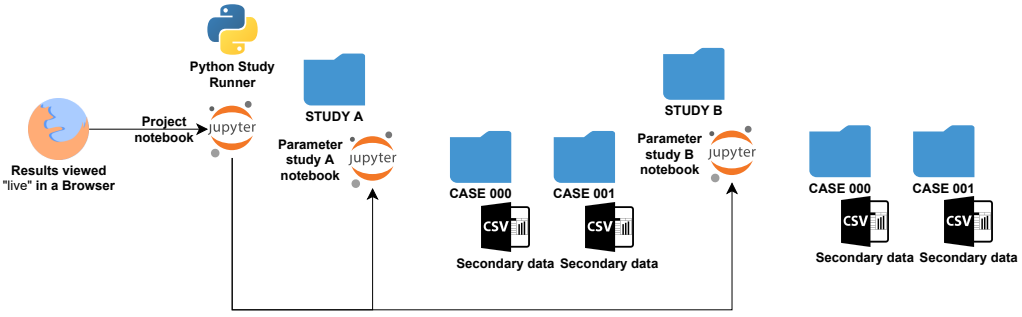
An example CI pipeline



A Research Software Engineering Workflow

Collecting the components: Parameter studies I

TECHNISCHE UNIVERSITÄT DARMSTADT

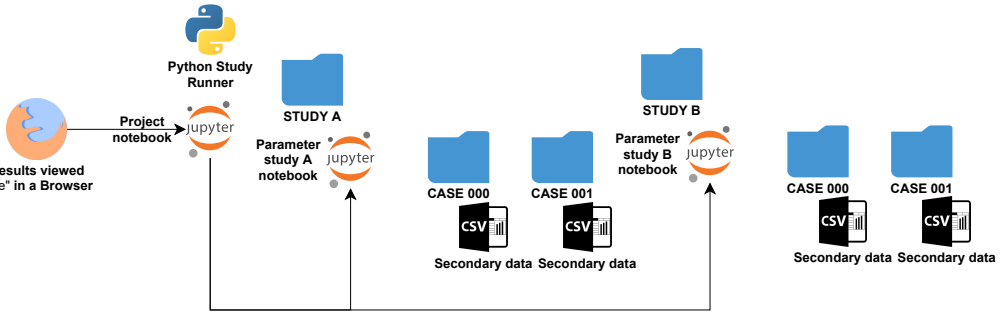


Organize your simulation studies.

A Research Software Engineering Workflow

Collecting the components: Parameter studies I

TECHNISCHE UNIVERSITÄT DARMSTADT



- Associate simulation cases with their metadata.
- `{case000 : {N_CELLS: 32, MODEL : shear2D}}`
- Store this information using a standard open-source format (**Interoperability** in FAIR).

TECHNISCHE UNIVERSITÄT DARMSTADT

Use Jupyter notebooks[2] and pandas[3] for

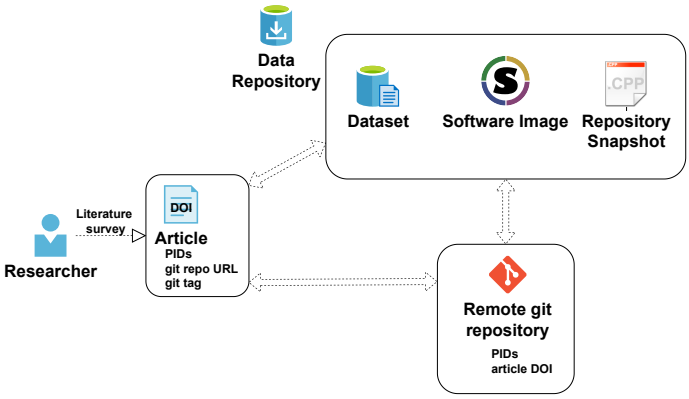
- **Documentation**: geometry, initial and boundary conditions, error norms, comparison data.
- **Data processing**: verification errors (conservation, convergence, stability), validation errors
- **Result analysis**: interactive and remote, while simulations are running!

[2] https://jupyter.org/
[3] https://pandas.pydata.org/

A Research Software Engineering Workflow

Collecting the components: Cross-linking

TECHNISCHE UNIVERSITÄT DARMSTADT



A Research Software Engineering Workflow

Collecting the components: Others

TECHNISCHE UNIVERSITÄT DARMSTADT

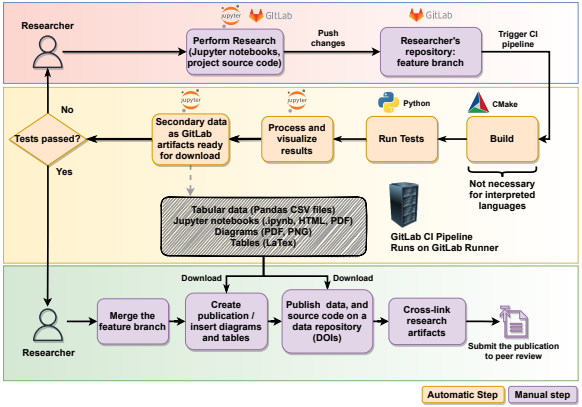
We did not cover in this talk:

- Build System and Containerization
- Test Driven Development (TDD)
- Continuous Benchmarking
- Regression Tests
- Parameter space exploration
- Metadata standard for secondary data
- Issue Tracking

A Research Software Engineering Workflow

Assembling the Workflow

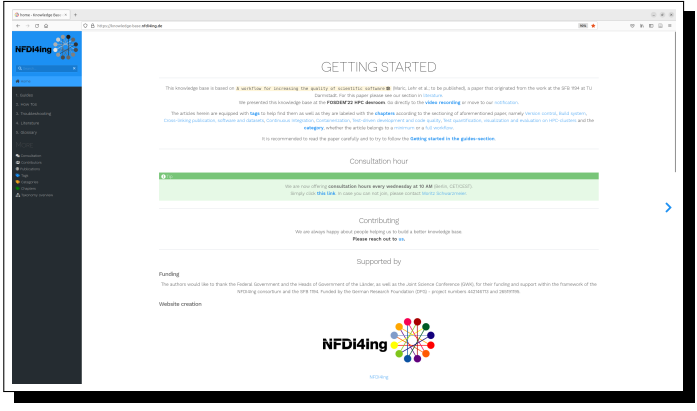
TECHNISCHE UNIVERSITÄT DARMSTADT




```
1:  Track changes using version-control.
2:  while Milestone not reached do
3:      for study in studies do            ▷ On an HPC cluster.
4:          Automate data processing and visualization.
5:          Run study.
6:          Check results and apply code changes.
7:      end for
8:      if results are improved on the HPC cluster then
9:          Push changes to the remote repository.
10:         if CI pipeline tests pass then
11:             Milestone reached.
12:             Add new tests to the CI pipeline,
13:             Merge feature into development branch.
14:             Cross-link publication, data, and source code.
15:         end if
16:     end if
17: end while
```

We run a Knowledge Base
that contains much more information

TECHNISCHE UNIVERSITÄT DARMSTADT



knowledge-base.nfdi4ing.de

Glossary terms display helpful information

when you hover over them

TECHNISCHE UNIVERSITÄT DARMSTADT

https://www.vecteezy.com/free-vector/mouse-pointer, Darmstadt, 21.01.2022

We just added interactivity
by offering a weekly consultation hour

TECHNISCHE UNIVERSITÄT DARMSTADT

The consultation hour is **every wednesday at 10 AM.**

- Information is displayed on the landing page.
- It is a **small initial investment**,
- but it **scales badly**.

We are curious, whether this will work out as:

- super-**interactive** for the users and
- super-direct **feedback** for us.

Let us know your opinion in the afterwards discussion!

Further reading

TECHNISCHE UNIVERSITÄT DARMSTADT

- This presentation
  is available at https://doi.org/10.5281/zenodo.7215818
- The **Knowledge Base**
  is available at https://knowledge-base.nfdi4ing.de
- **Preprint** describing the 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** about the workflow **at full length including hands-on**
  "Continuous" Integration of Scientific Software (in Computational Science and Engineering);
  Marić et al., 2021, https://zenodo.org/record/5522820.YnTOvnVByXI

Acknowledgements

TECHNISCHE UNIVERSITÄT DARMSTADT

Interaction between
Transport and Wetting Processes

Funded by the German Research Foundation (DFG) – Project-ID 265191195 –
CRC 1194 : Z-INF

Funded by the German Research Foundation (DFG) – Project-ID 442146713 –
NFDI4Ing : Base Service S-2 *Research software development*