A Workflow for Increasing the Quality of Scientific Software (in Computational Science and Engineering)

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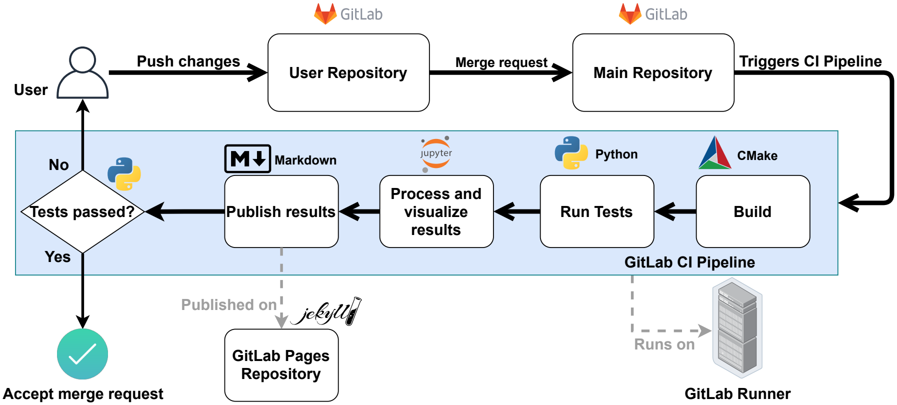
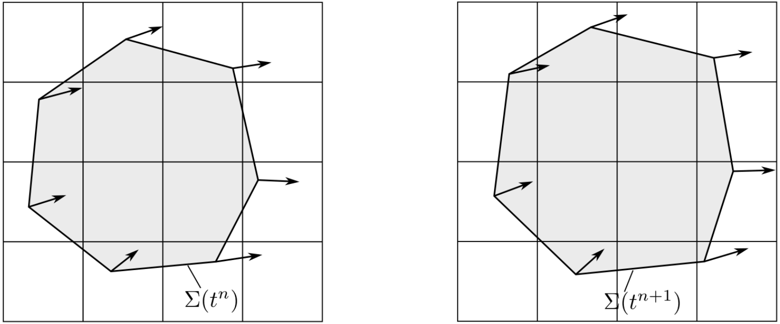
TECHNISCHE UNIVERSITÄT DARMSTADT



A Workflow for Increasing the Quality of Scientific Software (in Computational Science and Engineering) -
T. Marić, JP. Lehr, I. Pappagianidis, B. Lambie, D. Bothe, C. Bischof

Motivation: multiphase flow simulation software



- Fluids that do not mix are separated by an interface $\Sigma(t)$ (surface in 3D).
- Goal: track $\Sigma(t)$ as it moves in time t and changes its topology.

Motivation: multiphase flow simulation software

Lagrangian / Eulerian Interface Advection (LEIA) Methods

LEIA methods[1,2,3] require thorough testing:

- Verification cases: evolution of $\Sigma(t)$ and two-phase flows with exact solutions.
- Validation with respect to experiments.
- Serial and parallel computational efficiency.

[1] Marić, T., Marschall, H., & Bothe, D. (2015). lentFoam–A hybrid Level Set/Front Tracking method on unstructured meshes. Computers & Fluids, 113, 20-31.

[2] Tolle, T., Bothe, D., & Marić, T. (2020). SAAMPLE: A Segregated Accuracy-driven Algorithm for Multiphase Pressure-Linked Equations. Computers & Fluids, 200, 104450.

[3] Marić, T., Kothe, D. B., & Bothe, D. (2020). Unstructured un-split geometrical Volume-of-Fluid methods–A review. Journal of Computational Physics, 420, 109695.

Computational Science and Engineering software in university research groups

Boundary and initial conditions

- Publish or perish 🎓[4] prioritizes publications over scientific software.
- Dedicated resources for increasing software quality are usually not available.
- Ph.D. students rotate every 4-5 years, postdocs every 1-2 years.
  - Little or no overlap between successors and predecessors.
- Large-scale software design is not a necessary part of the CSE curriculum.
  - Different CSE background: (Applied) Mathematics, Mechanical Engineering, Physics, Informatics.
- Real-world example: onboarding people into ▸ OpenFOAM module development.

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

Computational Science and Engineering software in university research groups

Divergence

- Not being able to continue development from an earlier state.
- Reproducing results from a publication is not possible.
  - Data, source code and publication are not archived and cross-linked.
  - The version used to generate the data is not documented.
- Not being able to re-use a model from a publication.
  - The model is not implemented in a modular way.
  - Version integration was not done.
  - Non-granular commits were used.
- Having no overview of the impact of a change on the rest of the module.

A workflow for increasing the quality of scientific CSE software

1. Track the issues in a Kanban board.
   - Model issues as Progress Tracking Cards[5].
2. Use a simple version-control branching model.
3. Apply Test-Driven Development (TDD) for CSE software.
4. Enable Continuous Integration with an emphasis on result visualization.
5. Cross-link software, result data, and report/article when reaching a milestone.
   - When submitting a publication to peer-review.
   - After the publication has been accepted.
   - When giving up on an idea.
6. Bonus step: publish a Singularity image with the code and data.

[5] Developed by Better Scientific Software.

A workflow for increasing the quality of (academic) CSE software

OpenFOAM

The workflow is developed with OpenFOAM projects but it is tested with other software.

Disclaimer: This offering is not approved or endorsed by OpenCFD Limited, producer and distributor of the OpenFOAM software via www.openfoam.com, and owner of the OPENFOAM® and OpenCFD® trade marks.

Simple version-control branching model

Separation of Concerns and Single Responsibility

- University research teams *working on the same project* are generally small (2 - 5 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.
- OpenFOAM already uses object-oriented and generic software design patterns.

Simple version-control branching model

Change integration

Maintainers (postdocs, experienced Ph.D. students) manage the integration.

- Keep the branching model 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 *(CI)-tested improvements*.
  - **Feature**: SRP reduces git-conflicts with researchers working on different files.
- Complex branching workflow ⇒ complications with onboarding new members.

Test Driven Development

Program CSE tests first

TDD[6] for CSE

- Define verification and validation tests at the start.
- Focus placed the final result: interpolation, integration, discretization, PDE solution, physics.
- Top-down, instead of bottom-up test coverage.
- Don’t go overboard with unit-tests 🎓: extend unit-tests when debugging a failing CSE test.
- Focus kept on tests with real-world (publication) input.

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

Test Driven Development

Verification and validation tests define the Application Programming Interface

- **New code**: it is easier to program the API you wish for, if you are its first user.
  - Make the class interface easy to use correctly and difficult to use incorrectly[7].
  - Reduce number of function arguments, single responsibility, clear naming, ...
- **Legacy code**: extend existing API without modification.
  - OpenFOAM: understanding class hierarchies, *finding a base class with Runtime Type Selection and a virtual function to overload.*
- **The test application is the solver application with a different input.**
  - If possible, testing and solution is done by the same code.
  - This prevents code duplication.
  - Data output and additional checks can be disabled by (compile-time) options.

[7] Scott Meyers. 2014. Effective Modern C++: 42 Specific Ways to Improve Your Use of C++11 and C++14 (1st. ed.). O'Reilly Media, Inc.

Test Driven Development

Jupyter notebooks

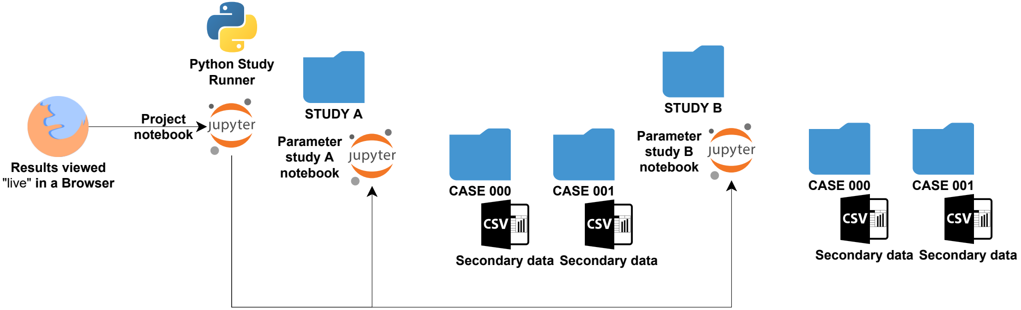
Jupyter notebooks[8]

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

[8] https://jupyter.org/

Test Driven Development

Parameter tests



Test Driven Development

Parameter tests: primary data (simulation results) organization

- The quality of CSE software is measured using verification and validation data.
- Effective comparison with others (previous versions) hinges on data organization.

- **Legacy code**:
  - use the existing folder structure and parameterization tools 🎓,
  - The mapping (case000) → (parameter vector) must be stored (YAML, ...)
- **New code**:
  1. Simple folder and file structure 🎓
  2. HDF5[9] or other open data format.
  3. Alternative to HDF5: **ExDir**[10]

[9] https://www.hdfgroup.org/solutions/hdf5

[10] Dragly, Svenn-Arne, et al. ”Experimental Directory Structure (Exdir): An alternative to HDF5 without introducing a new file format.” Frontiers in neuroinformatics 12 (2018): 16.

Test Driven Development

Parameter tests: secondary data (tables and diagrams) organization

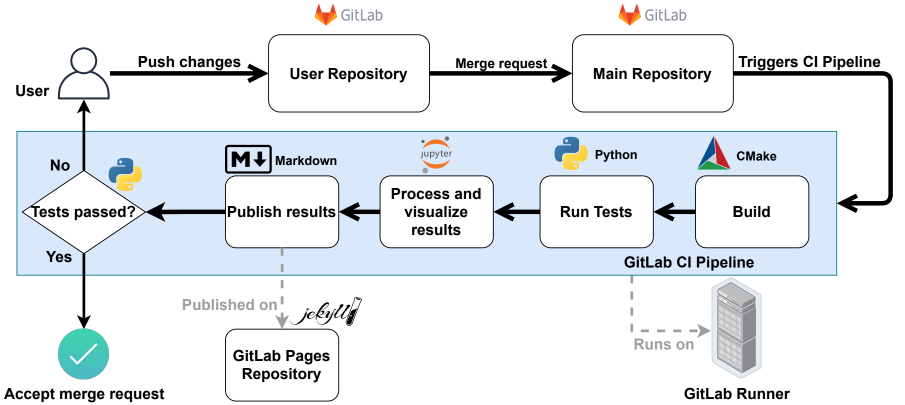
pandas.MultiIndex CSV with metadata for secondary data

- `pandas.MultiIndex` saved in ”metadata columns”.
- **Metadata is repeated**: not an issue for the small secondary data!
- Metadata in columns → `pandas.MultiIndex` → strongly simplified data analysis.
- **Direct readable export of tables to LaTex!**

	H	L_INF	O(L_INF)	EPSILON_R_EXACT_MAX	O(EPSILON_R_EXACT_MAX)
VELOCITY_MODEL					
SHEAR_2D	0.125000	0.032961	1.833407	0.032961	1.833407
SHEAR_2D	0.062500	0.009249	1.955529	0.009249	1.955529
SHEAR_2D	0.031250	0.002385	1.988745	0.002385	1.988745
SHEAR_2D	0.015625	0.000601	1.997178	0.000601	1.997178
SHEAR_2D	0.007813	0.000150	1.999294	0.000150	1.999294
SHEAR_2D	0.003906	0.000038	1.999294	0.000038	1.999294

Continuous Integration with result visualization

Schematic diagram



Continuous Integration with result visualization

Testing machines and test categorization

1. **Short few CPU-core tests**: work-PC 🎓.
2. **Short many-core tests**: obtain a workstation with a 64-Core CPU[11]🎓.
3. **HPC tests**: combine 1. or 2. with an HPC cluster.

An HPC cluster is relevant for production tests and performance measurements.

- This workflow uses coarse ("smoke") tests 🎓
  - Unit tests run for 1. and 2.
  - Convergence ensured for 1. and 2.
  - Is efficient in parallel for 1. and 2.
- **Challenge**: Is it possible to combine 1., 2. and 3. and publish instead of perish 🎓?

[11] Thanks to CRC 1194 at TU Darmstadt.

Continuous Integration with result visualization

A GitLab runner with a Docker executor and a local Docker image

Build a Docker image for your software, and track the Dockerfile with the project.

Example OpenFOAM Dockerfile on `ubuntu:focal` with ”system” open-mpi and scotch.

On the testing machine

- Install Docker and GitLab runner and register the GitLab runner with a Docker executor.
- Configure the GitLab runner in `/etc/gitlab-runner/config.toml` to
  - use a local Docker image, e.g., `image = "openfoam-v2012_ubuntu-focal:latest"`, and
  - never pull images `pull_policy = never`.

Continuous Integration with result visualization

Building

- Files created within a job are gone when the job ends.
- GitLab uses **job artifacts** to pass on data from one job to the next.
- **Job artifacts only work with 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

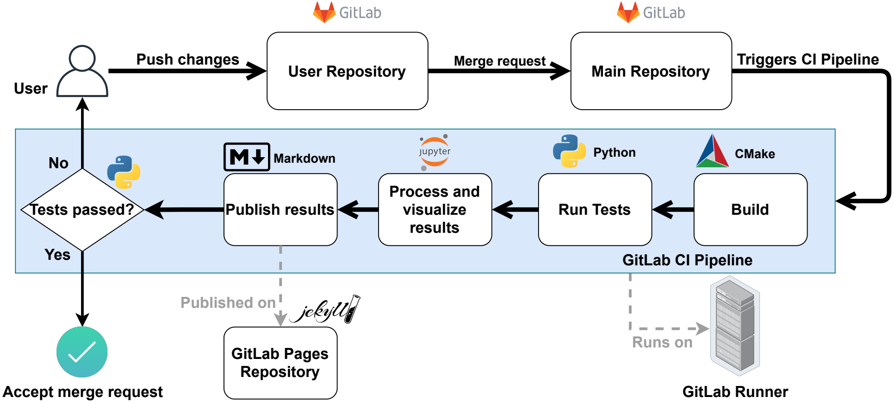
Building OpenFOAM projects or projects with out-of-source installation

Out-of-source installation: binaries only available outside the repo!

- **Use environment variables to build and pass on artifacts**
- `$FOAM_USER_LIBBIN` folder stores library binaries.
- `$FOAM_USER_APPBIN` folder stores application binaries.
- **Build job**:
  - create artifact folders inside the repo,
  - copy library and application binaries to artifact folders,
  - export artifact folders.
- **Run job: simplified copying of binary artifacts to OpenFOAM folders**
  - `mkdir -p {$FOAM_USER_LIBBIN, $FOAM_USER_APPBIN}`
  - `cp FOAM_USER_LIBBIN/* $FOAM_USER_LIBBIN`
  - `cp FOAM_USER_APPBIN/* $FOAM_USER_APPBIN`
  - Run tests.

Continuous Integration with result visualization

Schematic diagram



Continuous Integration with result visualization

Processing and visualizing results

```
jupyter nbconvert notebook.ipynb --execute --to FORMAT
```

- Execute each jupyter notebook in the repository.
- Notebooks agglomerate secondary data into `pandas.MultiIndex` CSV files.
- Export secondary data and notebooks in different formats as artifacts.
- **Visualization**
  - Download the artifact and open the notebook 🎓.
  - **Alternative:** publish the notebook as a blog post in a GitLab Static Page project.
  - Notebooks contain information on failing tests.
  - Mapping ”caseXYZ” → ”parameter vector” is crucial for re-starting failed parameter variations!

Continuous Integration with result visualization

Test evaluation

Very straightforward

- Python scripts test secondary data agglomerated by notebooks from simulation results.
- **Examples:**
  - Is the order of convergence of an error norm ≥ 2.0?
  - Is is the difference between simulation and experiment data $\leq 4\%$?

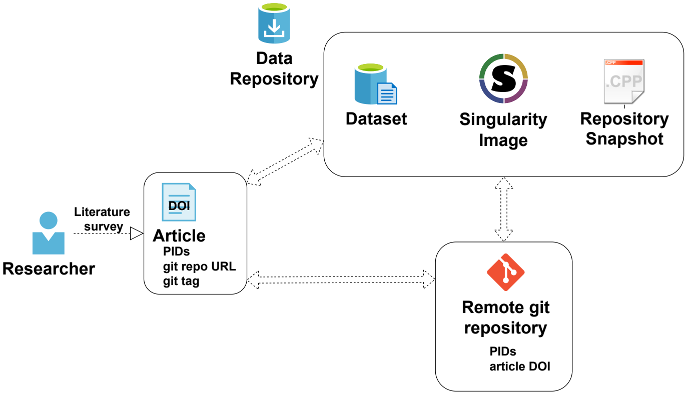
Continuous Integration with result visualization

Example

Example OpenFOAM CI project

Cross-linking data, source code and reports/publications

Schematic diagram



Cross-linking data, source code and reports/publications

Singularity

- Whence the Singularity Image[12]?
  - More intuitive than Docker: **Singularity handles images as files.**
  - Built for HPC from the start.
  - Doesn't require root rights.
  - Results as *actual files*, not "data in spinning containers".
  - Maps user folder to the container: result data remains on the host.
- Why not replace Docker with Singularity within GitLab CI?
  - We're learning how to do this using GitLab custom executors.
  - Does the workflow still survive publish-or-perish 🎓 test?
- Why a source-code snapshot on-top of the image and the repository?
  - Repositories get migrated, deleted, and some researchers still fear images.
  - Quick and direct access to source code from the publication.

[12] https://sylabs.io/docs/

Cross-linking data, source code and reports/publications

Singularity simplifies reproducibility

- The source code and the data stored in the image can be quickly reproduced.
- Article reviewers can clone, build, run and visualize easily.

Example: Singularity Image from an active review

- Clone the code repository from the image:
  ```
  geophase-JCOMP-D-19-01329R2.sif clone geophase
  ```
- Build:
  ```
  geophase-JCOMP-D-19-01329R2.sif build geophase build
  ```
- Run tests:
  ```
  geophase-JCOMP-D-19-01329R2.sif run-tests geophase build
  ```
- Open the jupyter notebook:
  ```
  geophase-JCOMP-D-19-01329R2.sif jupyter-notebook geophase
  ```

Similarity with other workflows / best practices

Our *(subjective)* estimates* of similarity $1 - 5$ (higher is more similar), $-$: aspect not addressed.

DOI	*Branching model*	*TDD*	*Cross-linking*	*CI*	(Meta)data standardization
10.12688/f1000research.11407.1	-	-	-	-	1
10.3934/math.2016.3.261	-	-	-	-	2
10.1371/journal.pbio.1001745	1	2	-	-	-
10.1371/journal.pcbi.1005510	-	-	3	1	3
10.1145/2723872.2723881	1	-	-	1	-
10.1145/3324989.3325719	1	-	-	5	-
10.1371/journal.pone.0230557	1	-	-	1	4
10.1145/3219104.3219147	1	-	-	4	-

*The list may still be incomplete.

Lessons learned

- Keeping the workflow as simple as possible is crucial for acceptance.
- Focusing on secondary data simplifies the workflow significantly.
- For simulations that run < 24 hours primary data can be recomputed easily.
- Periodical cross-linking of research data is done quickly and it is very beneficial.
- Personal responsibility is crucial at University research groups: who are the maintainers?
  - What are the incentives for maintainers?
- Fixing the (parallel) I/O of legacy scientific codes requires a large amount of effort.
  - It should be done outside of research projects.

Outlook

- Performance CI jobs run on 64-core workstations: moving on to the HPC cluster.
- Singularity GitLab executor?
- Jupyter Hub for interactive analysis of problems in parameter variations?
- Automatic publishing and cross-linking of CI artifacts?
  - Source code archive, Singularity container, secondary data.
  - Data repository API must be used to modify metadata.

Acknowledgements

CRC 1194

Interaction between
Transport and Wetting Processes

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