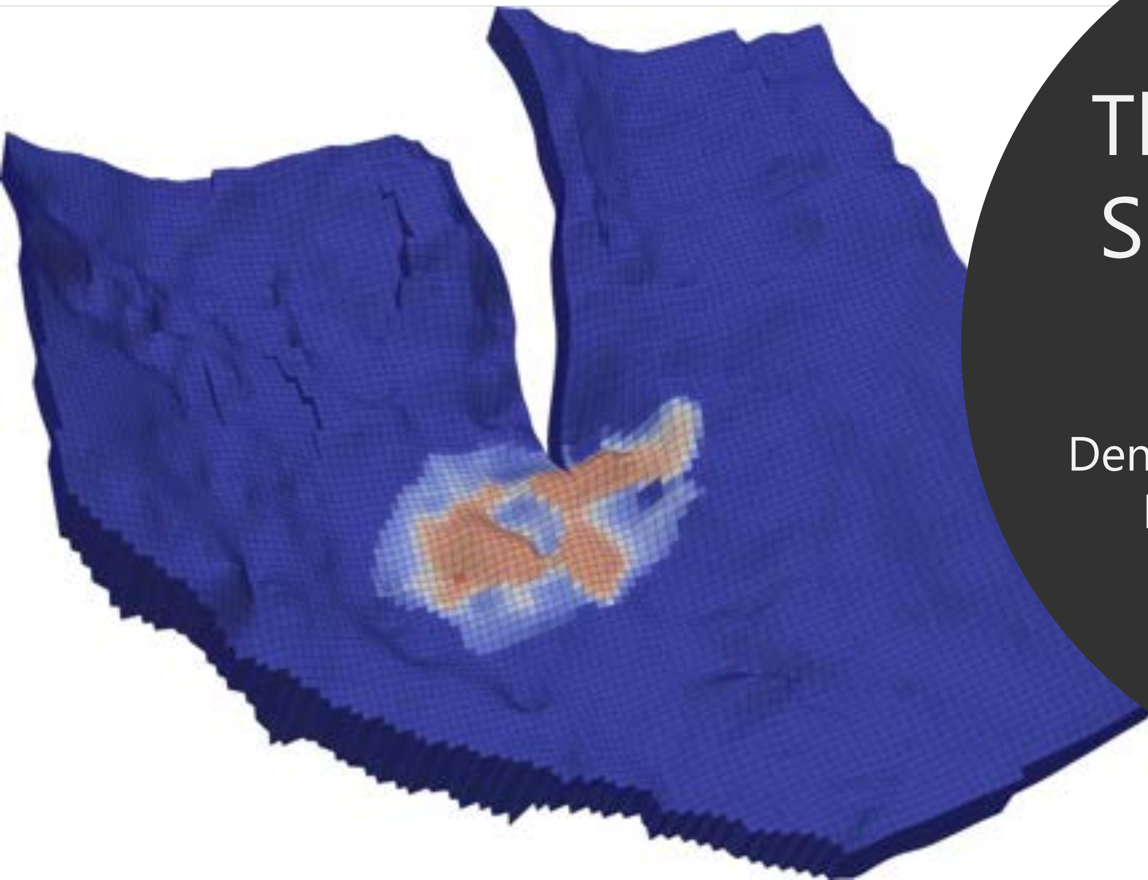
University of Stuttgart
Institute for Modelling Hydraulic and Environmental Systems
Department of Hydromechanics and Modelling of Hydrosystems

DuMu^X



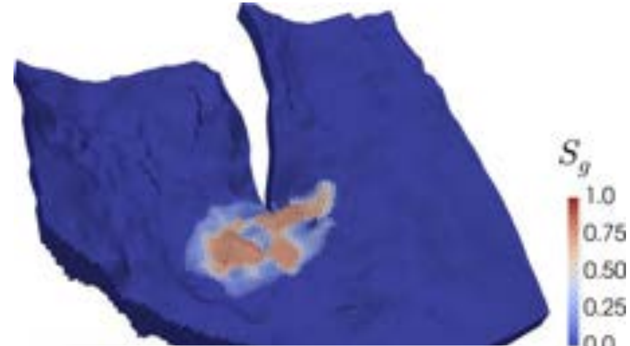
The Open-Source Simulator DuMu^x

Bernd Flemisch,
Dennis Gläser, Timo Koch and the
DuMu^x development team

DARTS Workshop
TU Delft, 07.03.2023

LH²

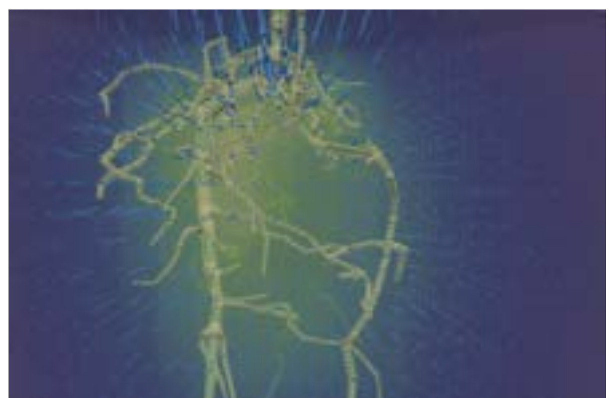
Coupled free- and porous-medium flow



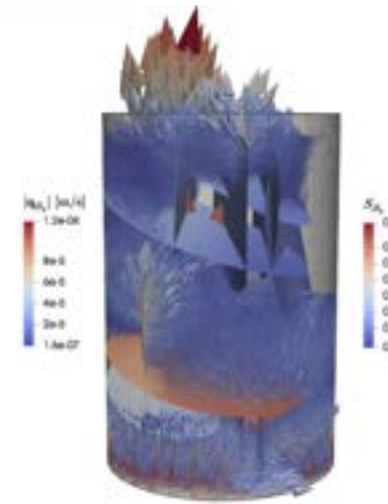
Subsurface gas storage

DuMu^X

River engineering



Root-soil interaction



Fracture flow

Outline

Overview

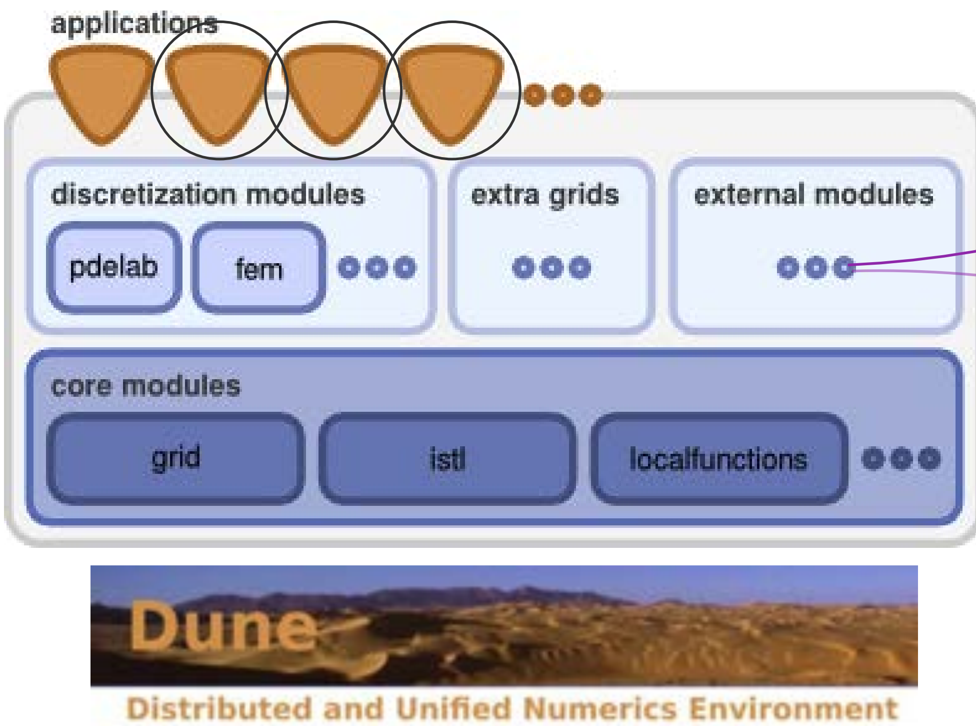
Development

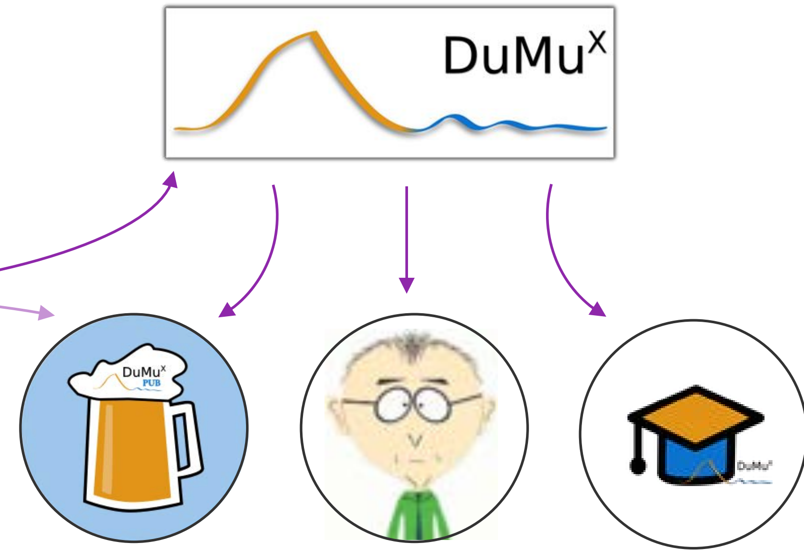
Quality Assurance

Verification &
Validation

Reproducibility

DuMu^x as an external Dune module





Available Models

Porous Medium Flow: Fully Implicit	Porous Medium Flow: Sequential	Free Flow: Fully Implicit	Geomechanics: Fully Implicit	Multidomain: Fully Implicit
1p, 1p2c Richards	1p + tracer	stokes navierstokes rans (0-Eq, 2-Eq)	el1p2c	Boundary: Darcy-Darcy, Stokes-Darcy
2p, 2p1c, 2p2c, 2pdfm, 2pminc, 2pnc, 2pncmin, co2	2p + tracer		el2p elastic	Facet: Darcy-Darcy 1/2d-2/3d
3p, 3p3c, 3pwateroil				Embedded: Darcy-Darcy 1/2d-3d
mpnc				
+ non-isothermal	**+ non-isothermal**	**+ compositional** **+ non-isothermal**		

Further Capabilities and Characteristics

Porous Medium Flow

Fully Implicit

Discretization:

- Box method
- Cell-centered FV with TPFA or MPFA

Grid Adaptivity ☑

Parallel ☑

Sequential

Discretization:

- Box method
- Cell-centered FV with TPFA or MPFA

Grid Adaptivity ☑

Parallel ☑

Free Flow

Fully Implicit

Discretization:

- Staggered grid (MAC) method

Geomechanics

Fully Implicit

Discretization:

- Cell-centered method for flow
- Box for displacement

Parallel ☑

Multidomain

Fully Implicit

Discretization:

- Stokes-Darcy: cell-centered for PM flow, staggered for free flow
- …

Status quo

- Main **user base** at the LH2, but there are considerably many external users
- Almost all of the **development** is done at the LH2, occasional external contributions
- Almost all developers have an **engineering background** with little experience in SD
- **> 70 contributors** so far
- 2961 version-controlled **files**
- 566 **tests,** the majority being regression tests by means of small simulations
- **Documentation:**
  - Website
  - Doxygen
  - Handbook
  - Course material

Outline

Overview

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Quality Assurance

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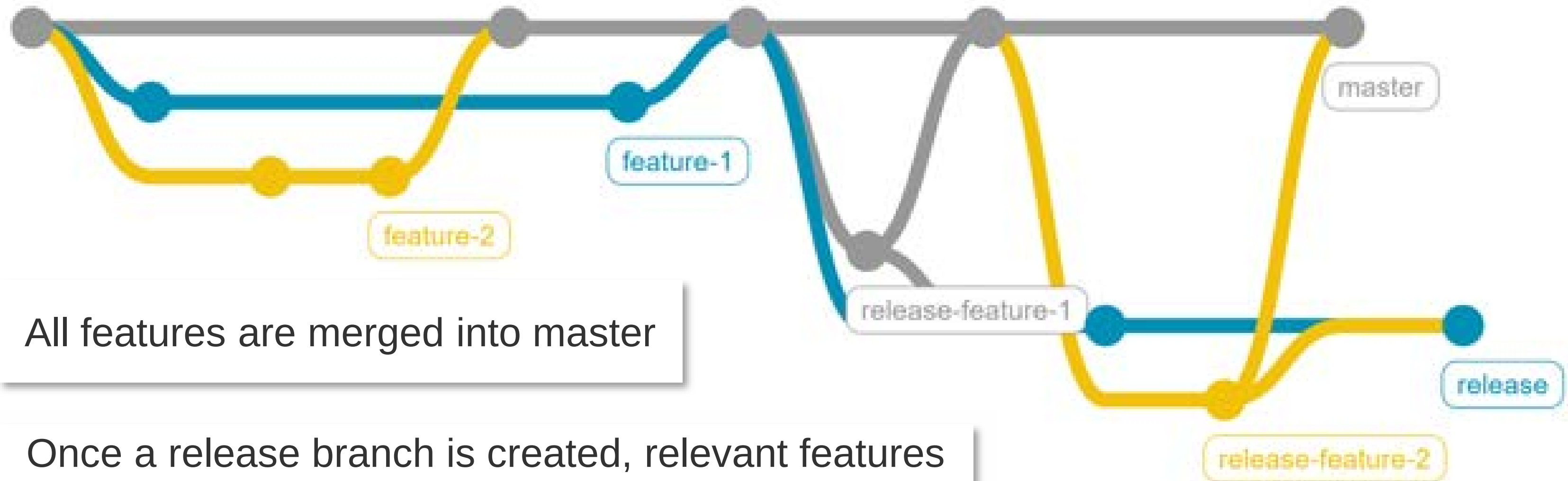
Validation

Reproducibility

Development process

Git workflow



All features are merged into master

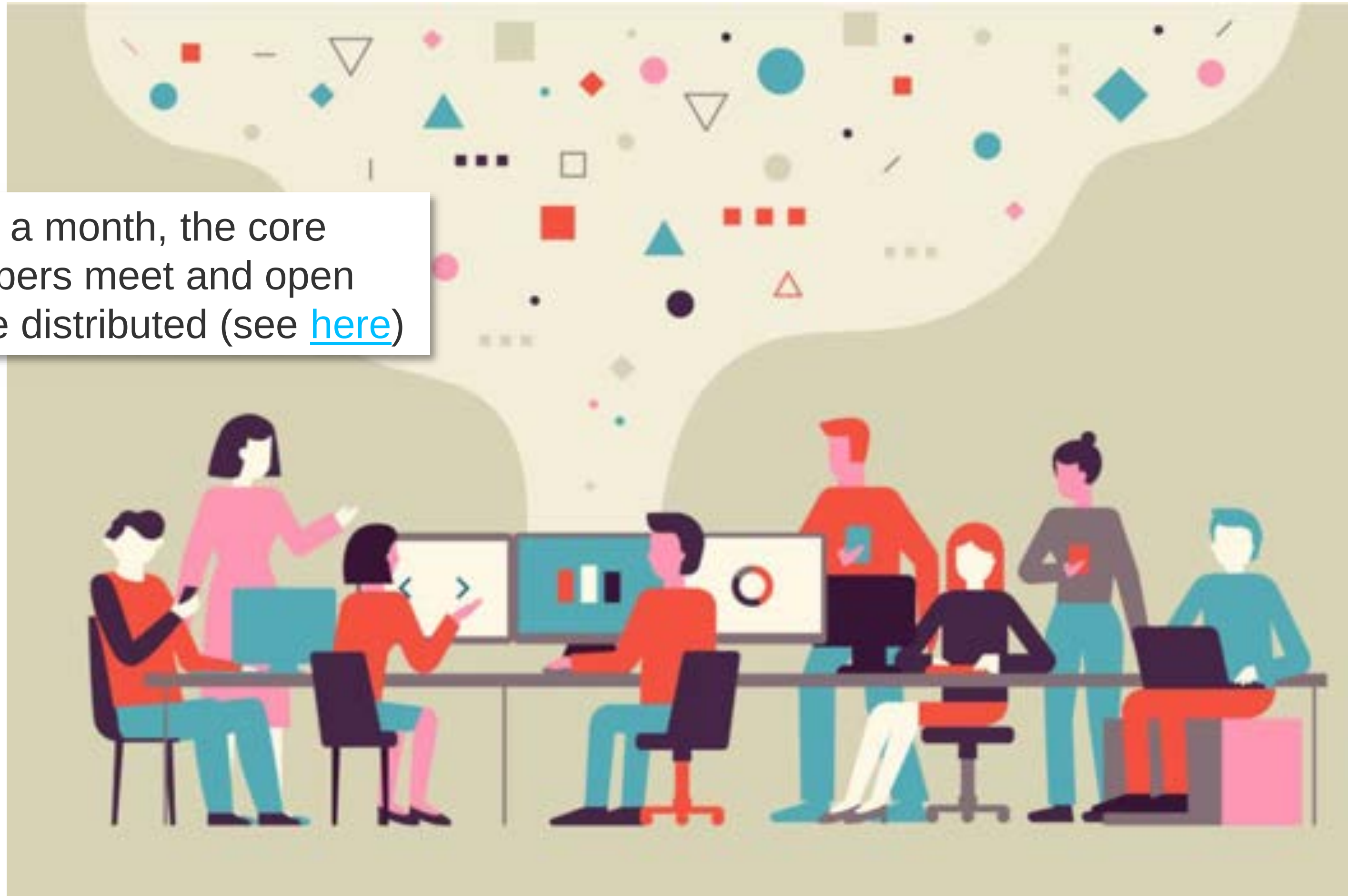
Once a release branch is created, relevant features are merged into both master and release

Release branches are maintained after release, bugfixes are backported

Rebase required before merging is possible (not depicted in the image above)

Development process

DuMu^x Days



Once a month, the core developers meet and open issues are distributed (see here)

Development process

Releases

A release manager is assigned for each release

The release manager tasks are listed in a GitLab Issue template (see e.g. here)

Outline

Overview

Development

Quality Assurance

Verification & Validation

Reproducibility

Quality assurance

Merge requests: guidelines shown in default template

Choose a template

Write | **Preview**

What this MR does / why does DuMux need it:

TODO: insert text here

Notes for the reviewer

TODO: insert text here

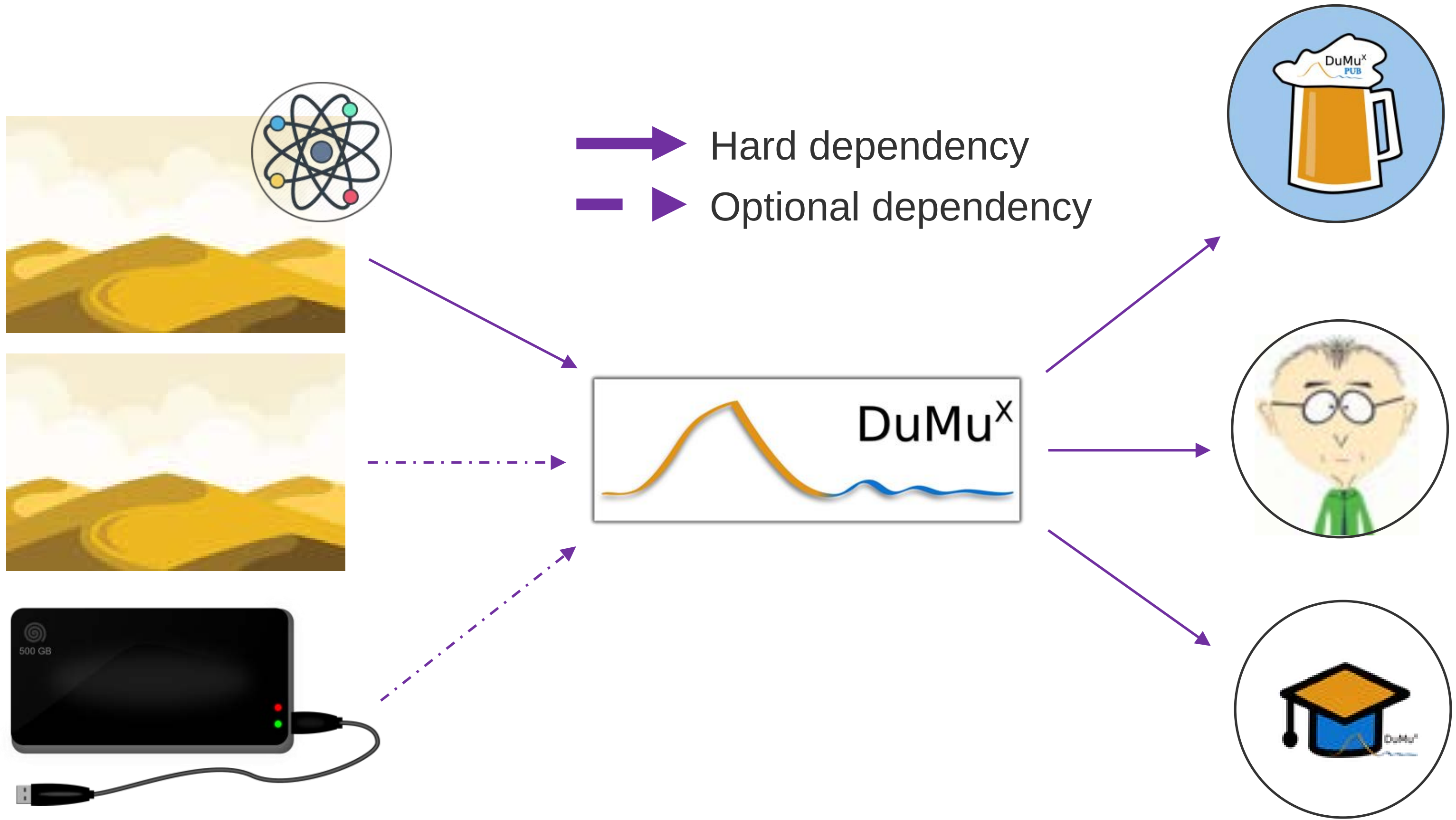
Before you request a review from someone, make sure to revise the following points:

- [ ] does the new code follow the style guide?
- [ ] do the test pipelines pass? (see guide on how to run pipelines for a merge request)
- [ ] is the code you changed and/or the new code you wrote covered in the test suite? (if not, extend the existing tests or write new ones)
- [ ] does your change affect public interfaces or behavior, or, does it introduce a new feature? If so, document the change in `CHANGELOG.md`.
- [ ] is the list of the header includes complete? ("include what you use")
- [ ] all files have to end with a `\n` character. Make sure there is no `\ No newline at end of file` comment in "Changes" of this MR.
- [ ] (if not applicable remove) are newly introduced or modified physical values/functions backed up with a scientific reference (including doi) in the docs?
- [ ] (if not applicable remove) if the examples are modified, is the documentation regenerated (using `generate_example_docs.py`)

Closes #1054 (closed)

Quality assurance

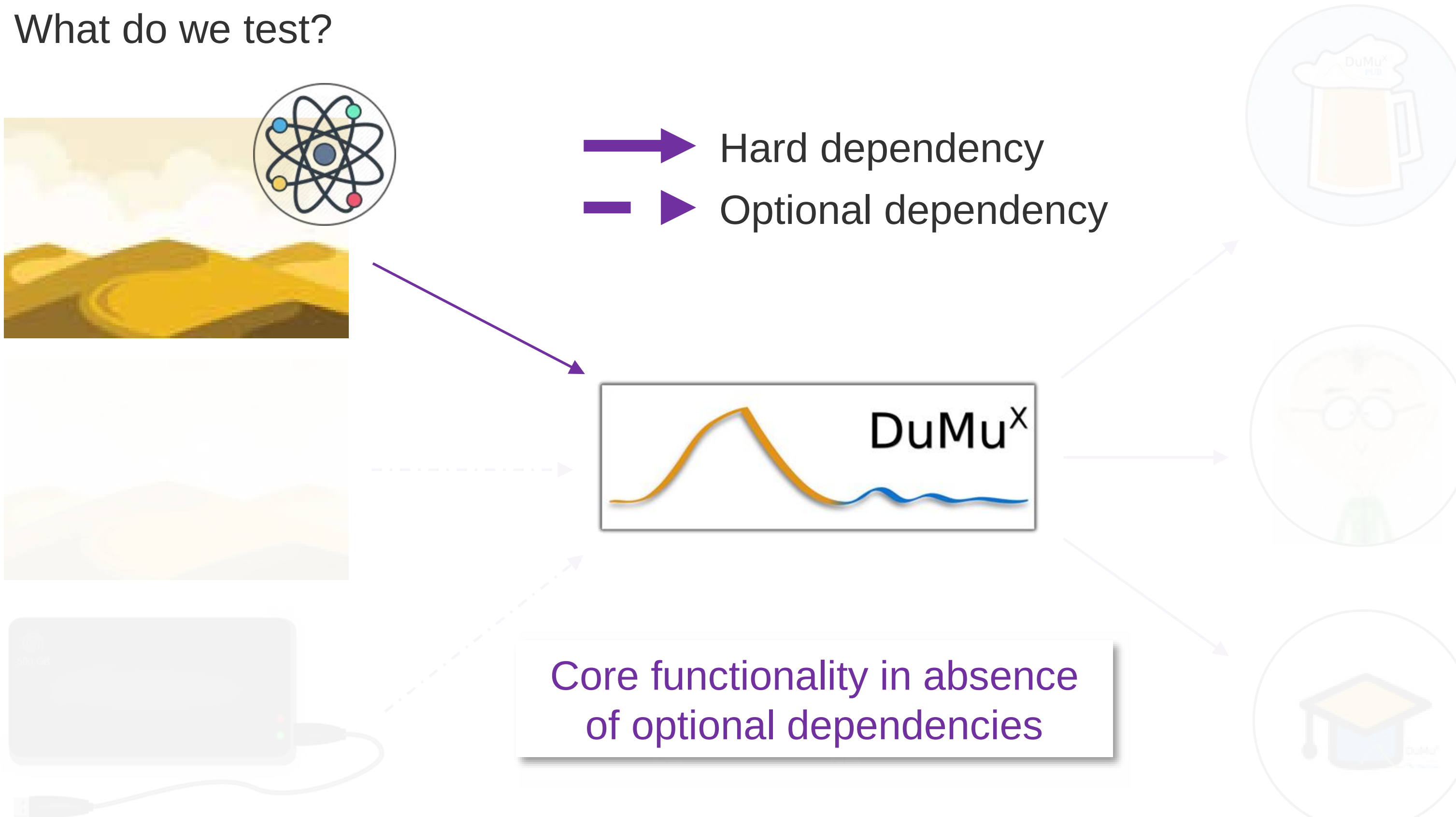
Test pipelines



Quality assurance

Test pipelines

- What do we test?

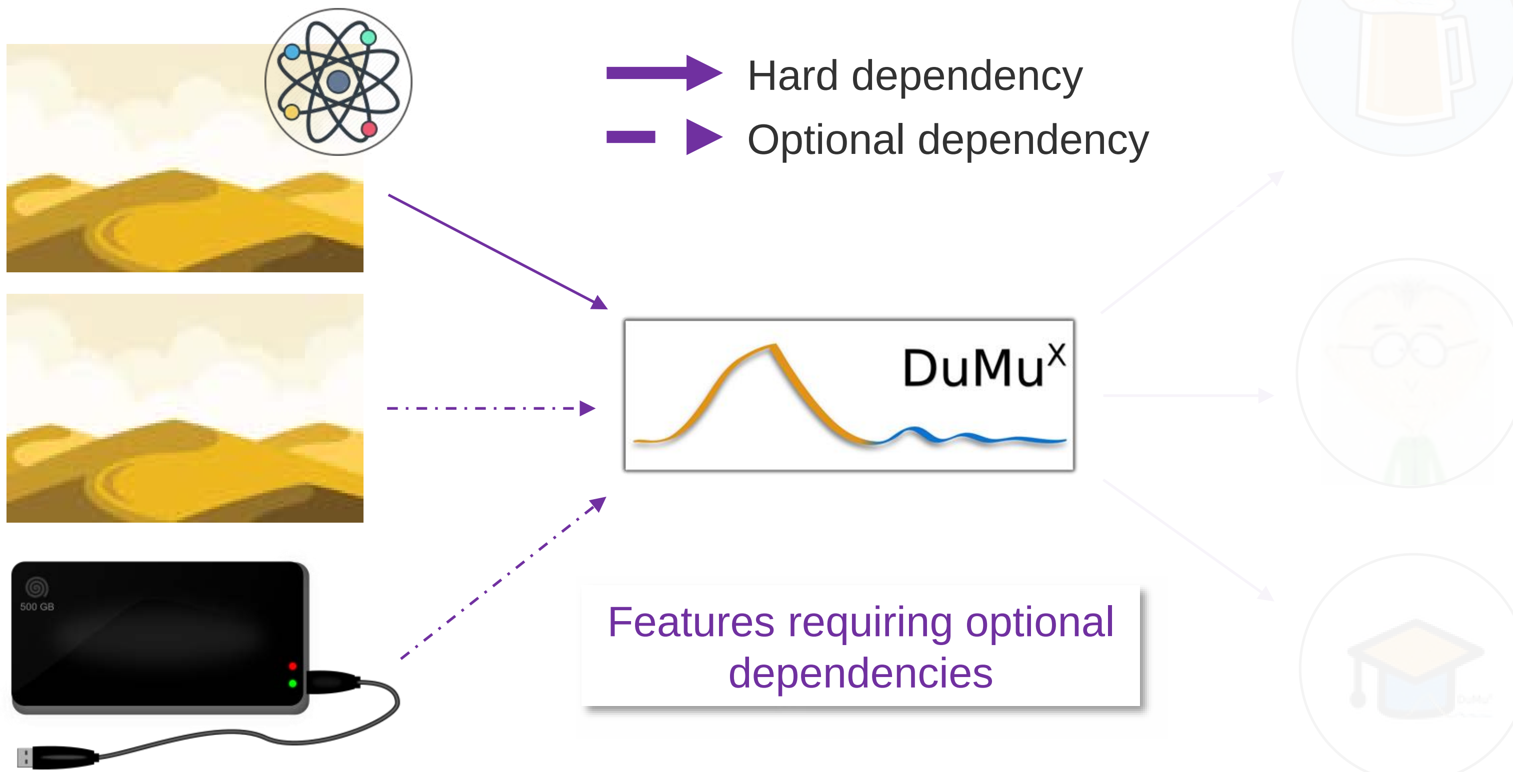


Core functionality in absence of optional dependencies

Quality assurance

Test pipelines

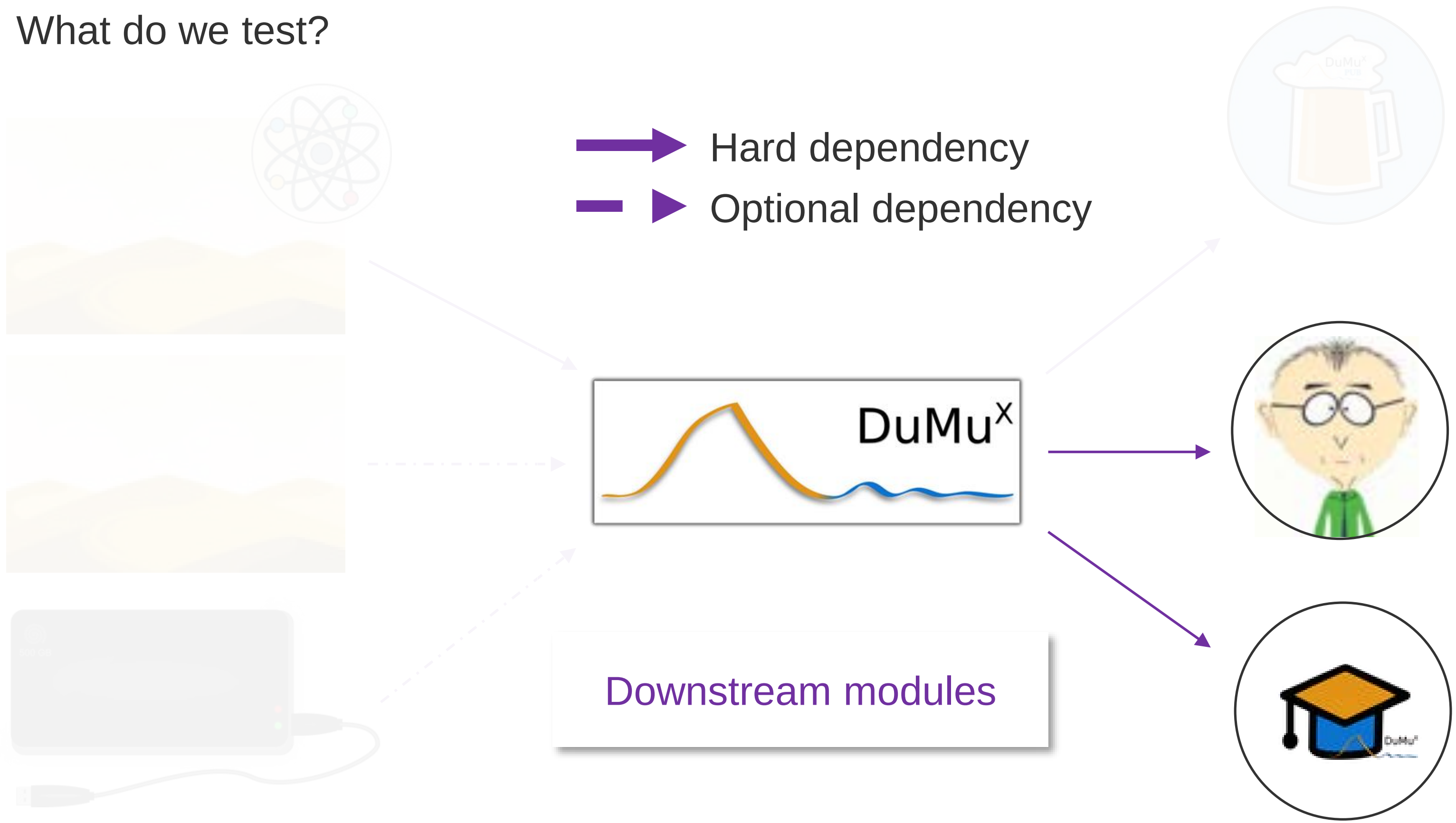
- What do we test?



Quality assurance

Test pipelines

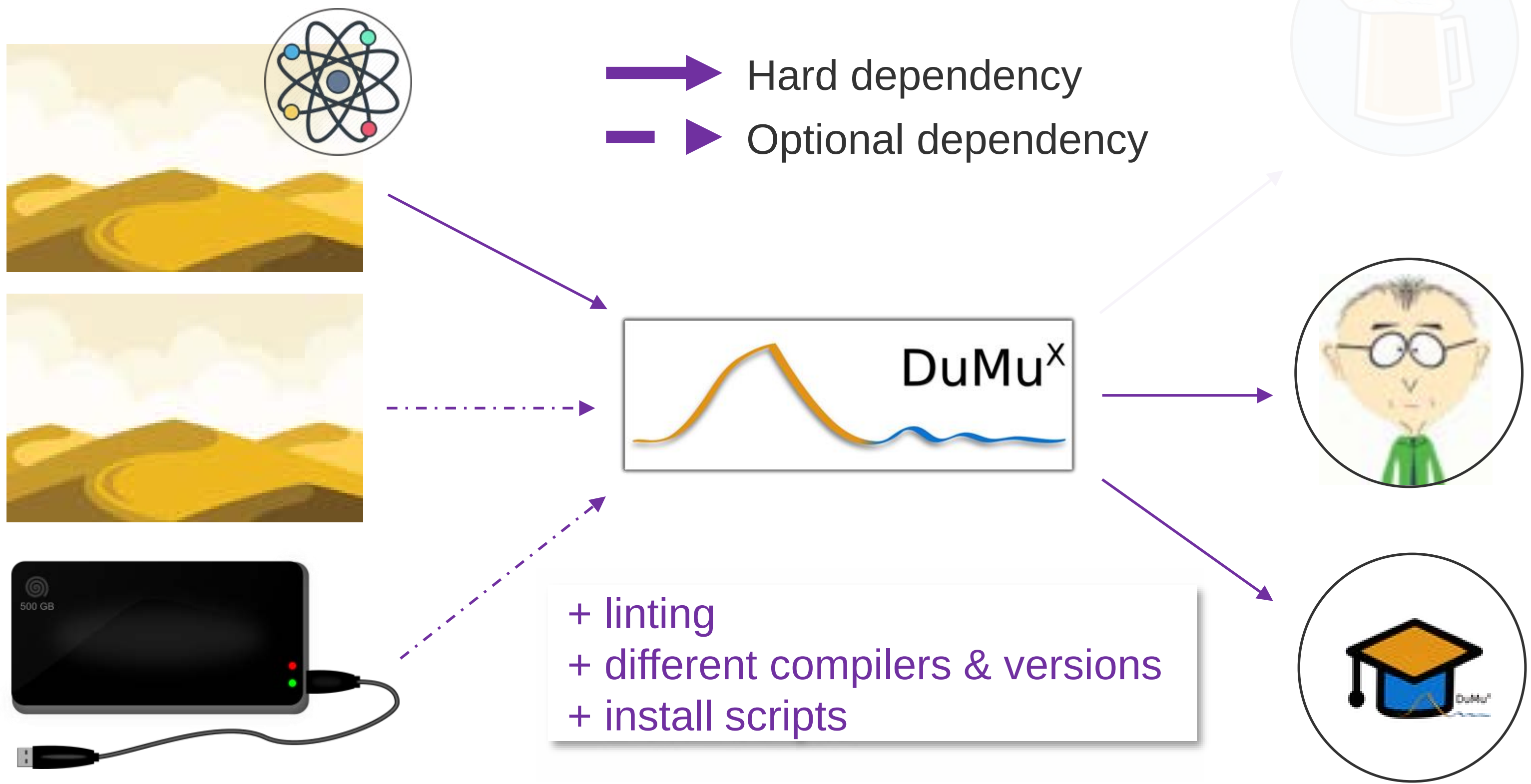
- What do we test?



Quality assurance

Test pipelines

- What do we test?

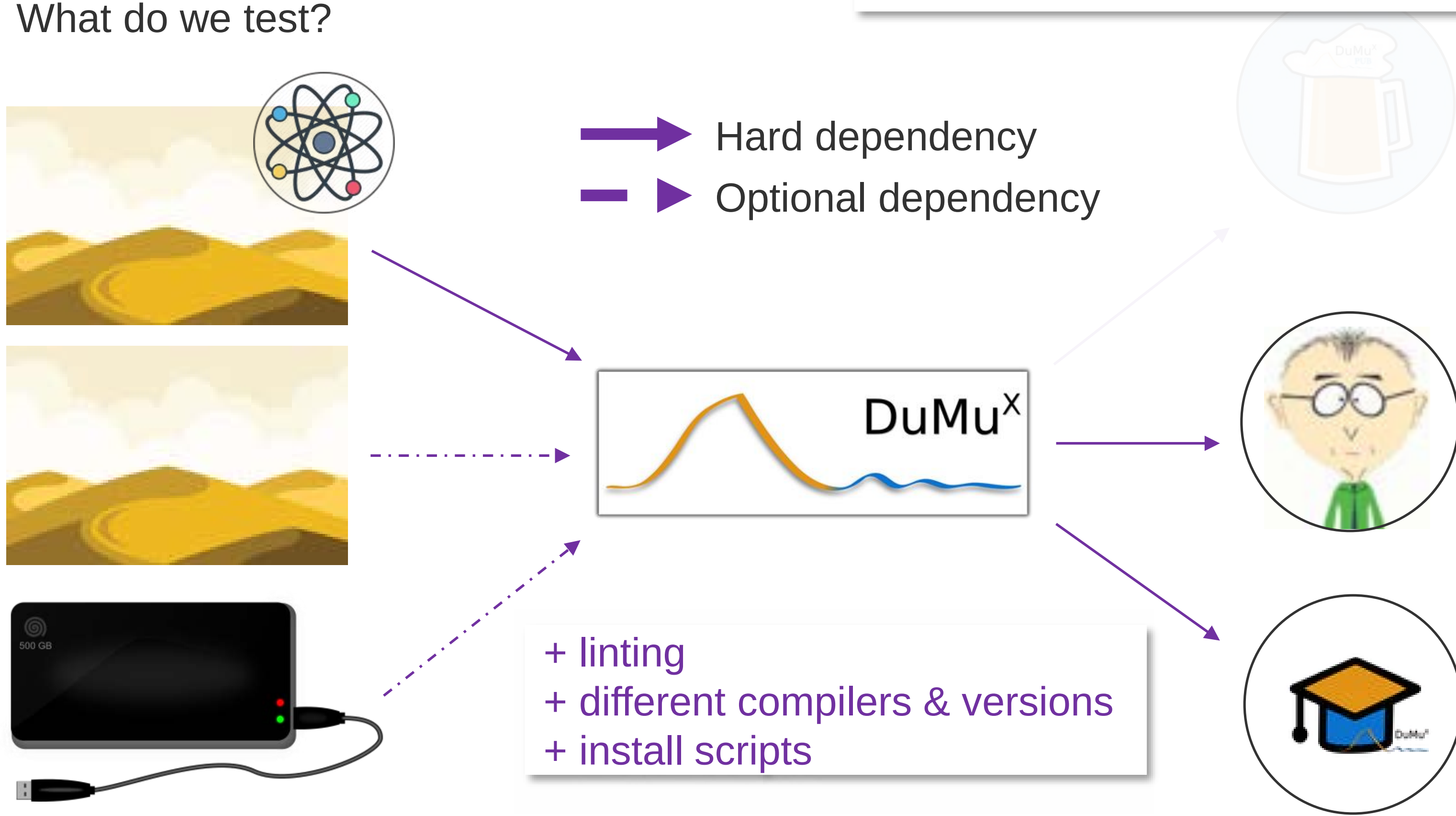


Quality assurance

Test pipelines

git.iws.uni-stuttgart.de/dumux-repositories/dumux/-/pipelines/21181

- What do we test?



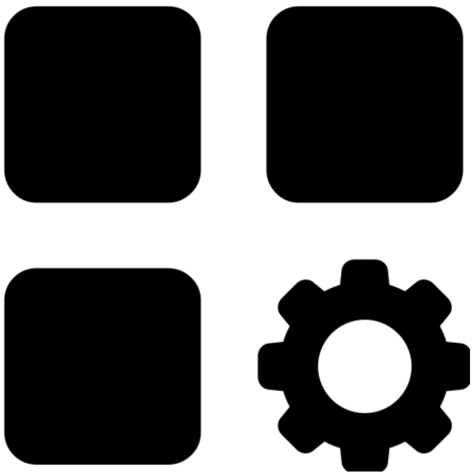
Quality assurance

Test pipelines: saving CPU time

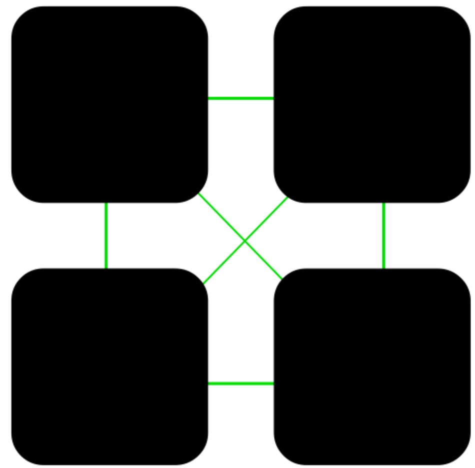
- “Problem”: very many tests that take several hours to compile (on a single core)
- Solution strategy:
  - Run only the tests that are affected by changes since the last successful run
  - Only schedules run the entire test suite
  - An example: git.iws.uni-stuttgart.de/dumux-repositories/dumux/-/pipelines/20820

Quality assurance

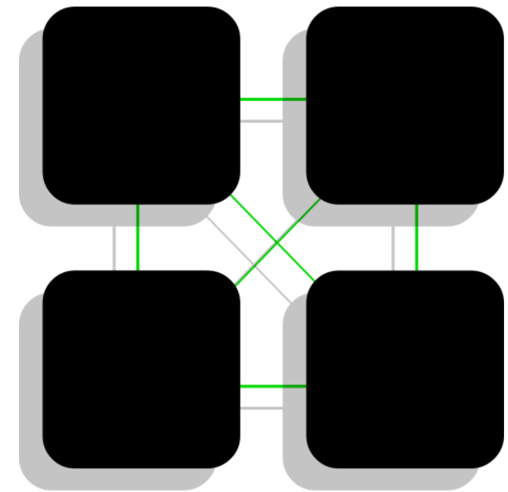
Test characteristics



Unit tests



Integration tests



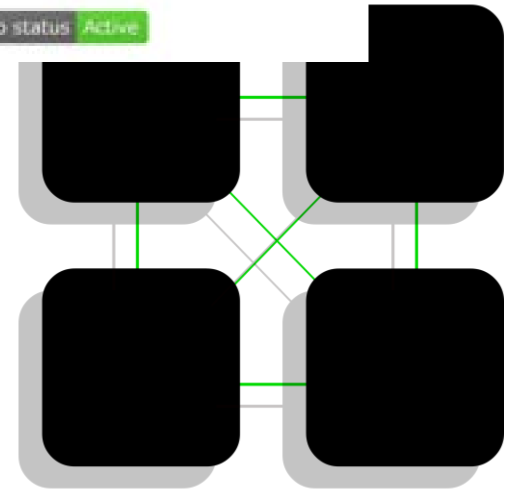
Regression tests

Quality assurance

Testing simulations

gitlab.com/dglaeser/fieldcompare

- Regression tests in Dumux:
  - Short simulations with a specific model
  - Comparison of the simulation results against reference solutions that were obtained earlier
  - Deviation in the results causes the test to fail
  - After bugfixes, reference results may be updated



Regression tests

\+ **Developers notice when a change in the code changes the physics**

− **The test says nothing about the “physical correctness” of the model**

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Selected Benchmark Study

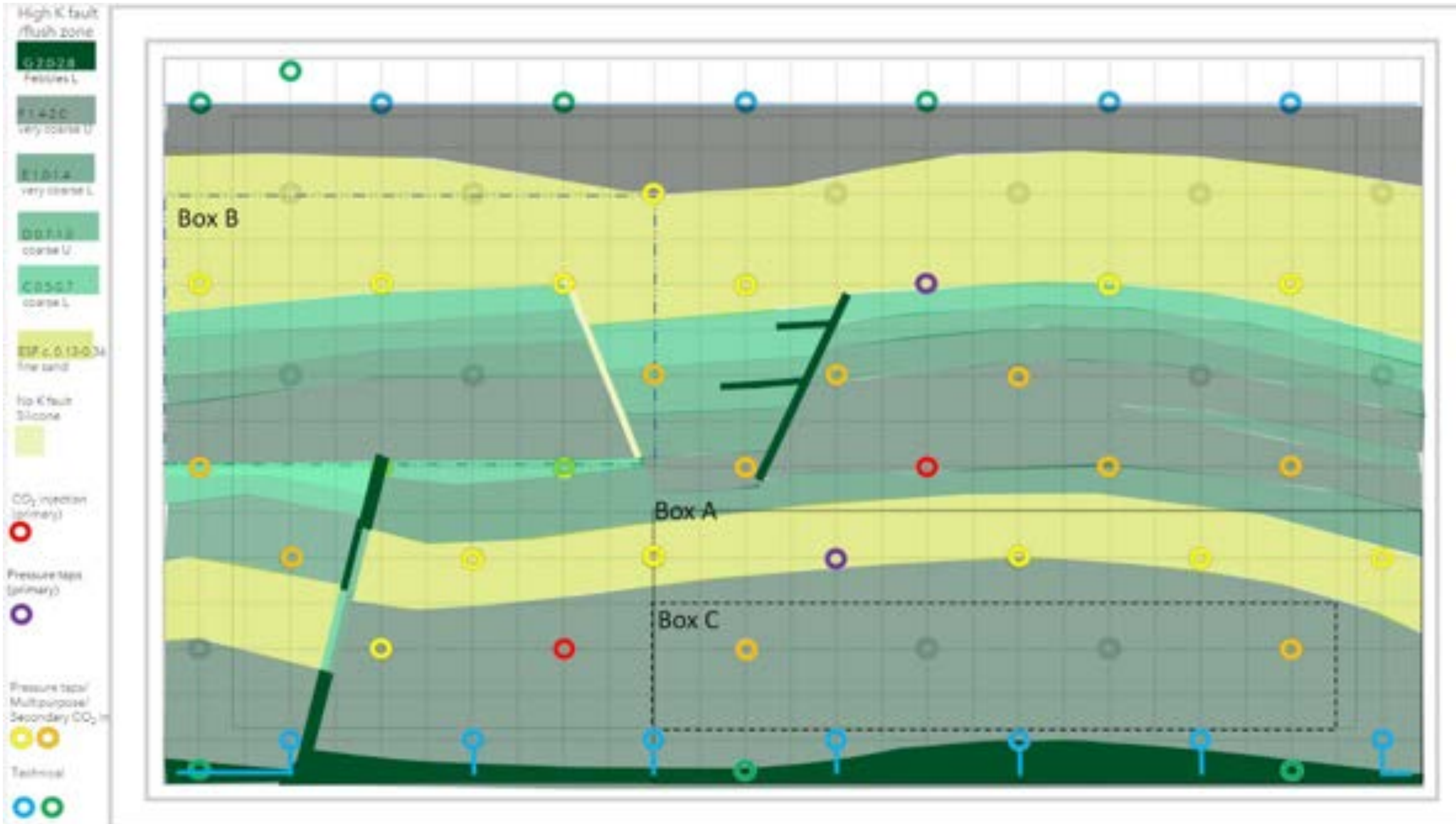
FluidFlower International Benchmark Study (2023)

- Validation
- Invitation-only, multi-stage blind/open process
- 9 groups, 9 models
- Data from **6 experimental runs**
- SRQs:
  - Saturation and concentration fields at selected time steps
  - Integrated phase composition … over time
  - **Mean and std dev** for various quantities
- Metrics: Wasserstein distance, …
- Other reported characteristics: Model assumptions, implementation details, …

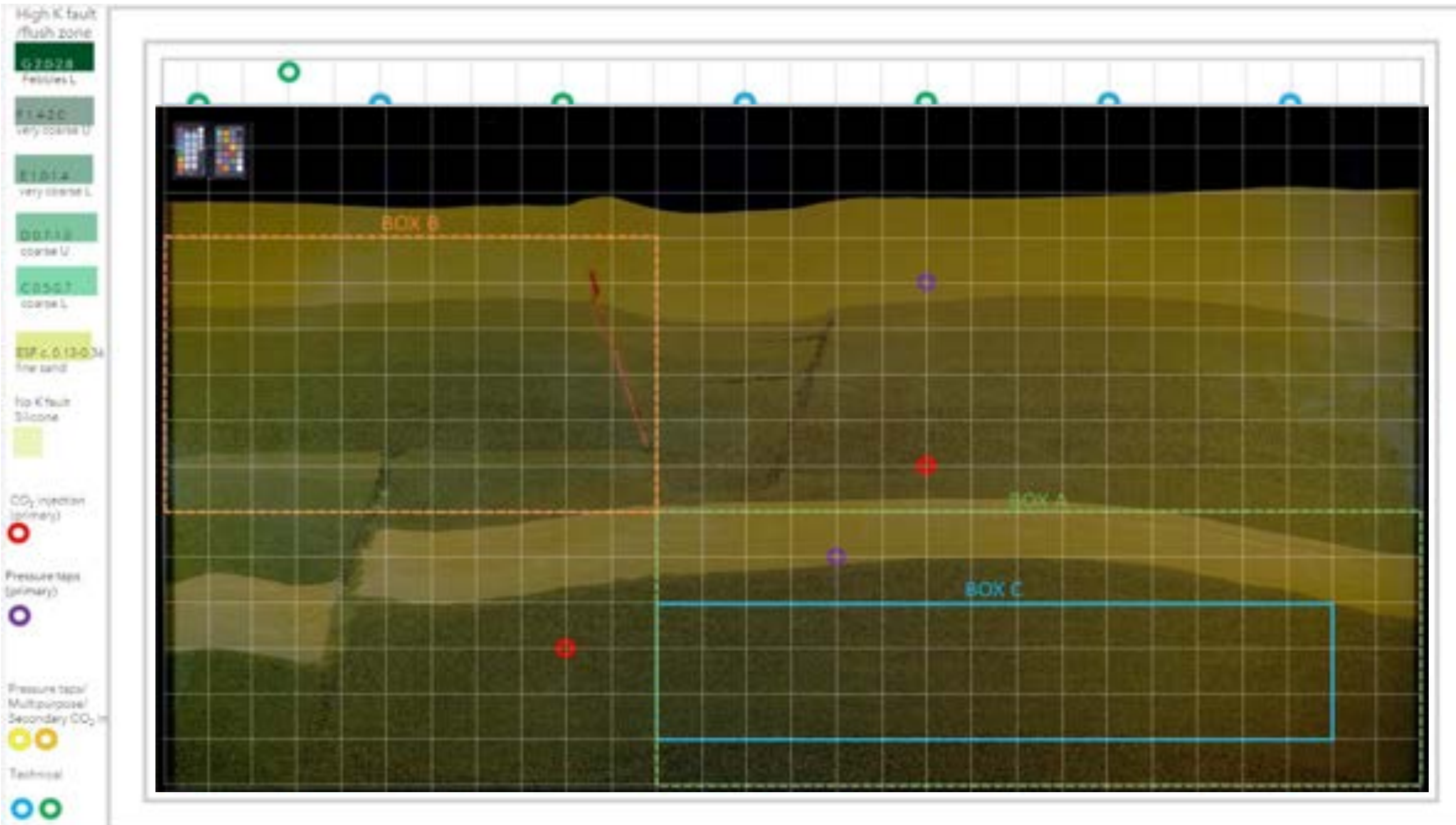
J. Nordbotten, M. Fernø, B. Flemisch, R. Juanes (eds.) (2023): “FluidFlower: modeling, simulation, and prediction of complex multiphase flow systems“, *TiPM Special Issue (planned)*.

Experimental Rig

Intended Geometry

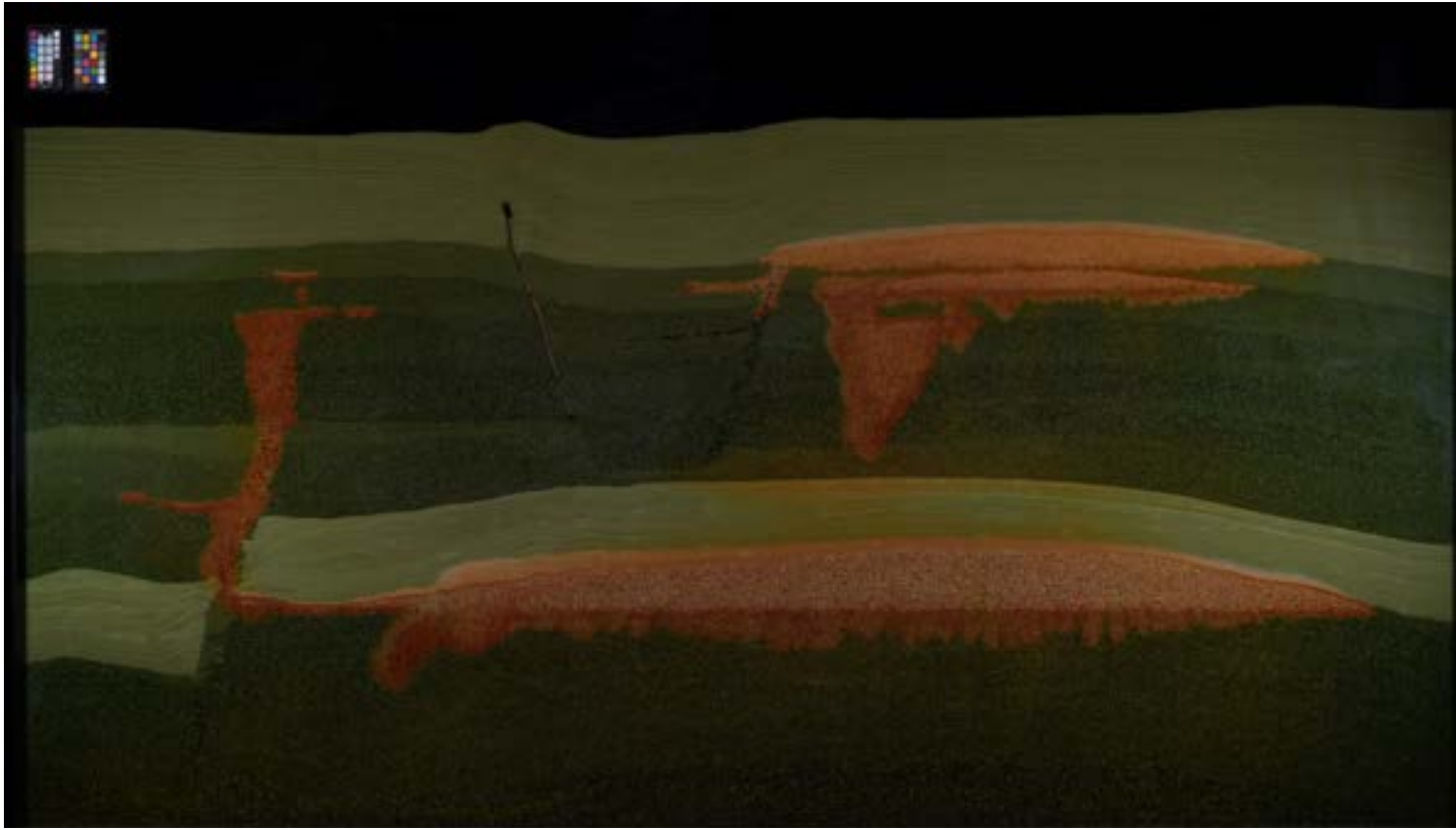


Implemented Geometry



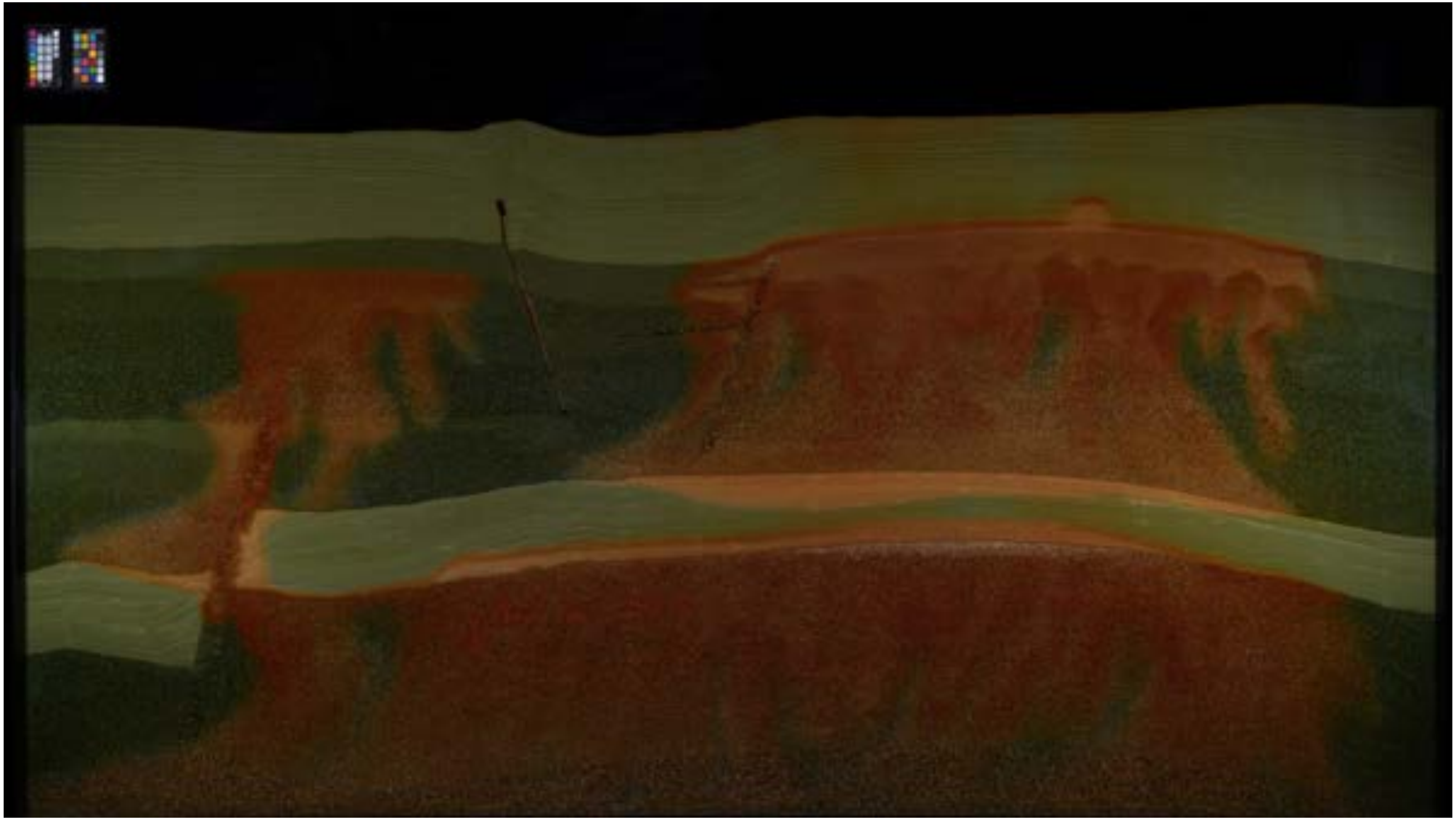
FluidFlower International Benchmark Study (2023)

Snapshot after 240 Minutes = 4 Hours



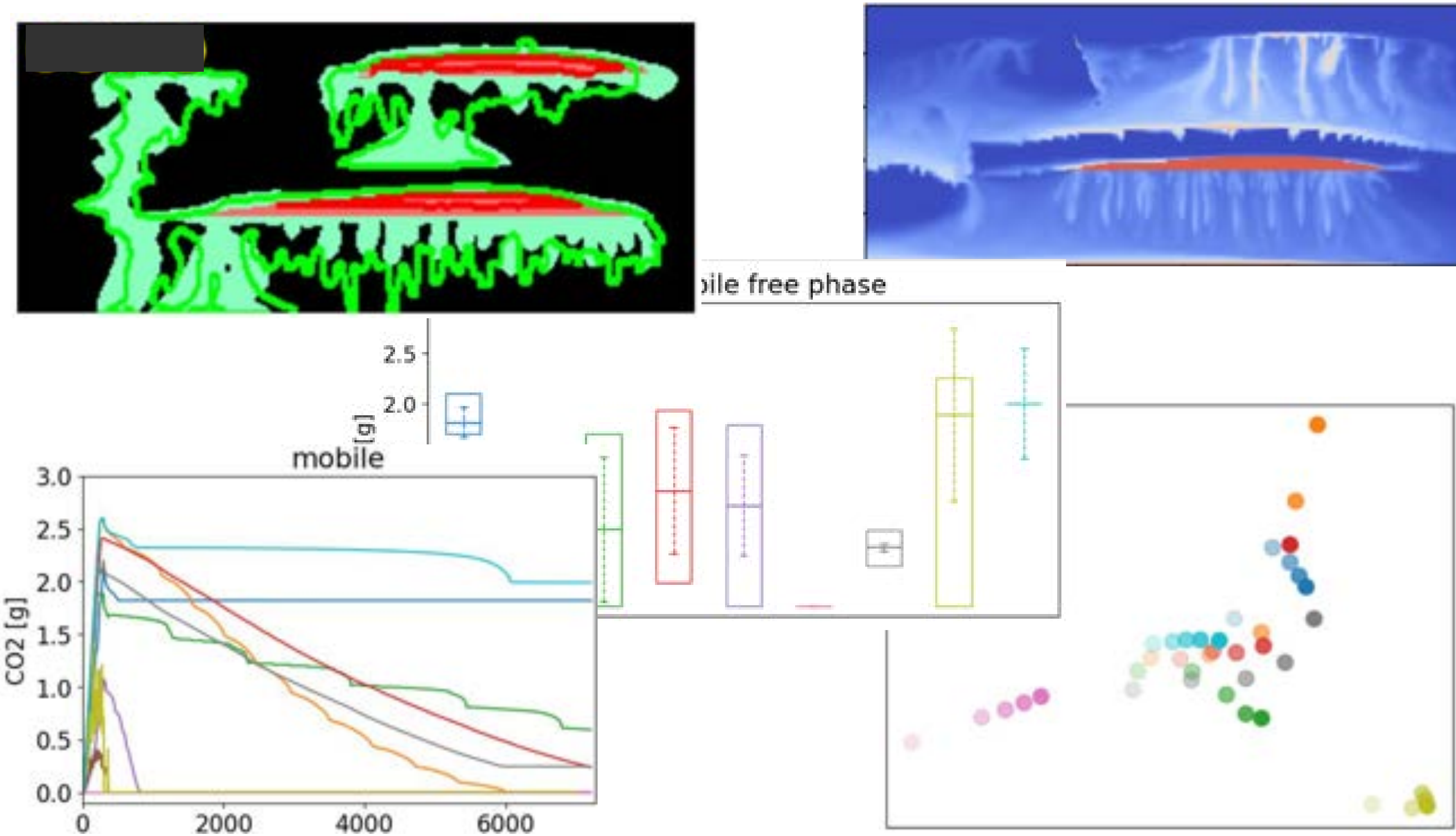
FluidFlower International Benchmark Study (2023)

Snapshot after 4320 Minutes = 72 Hours



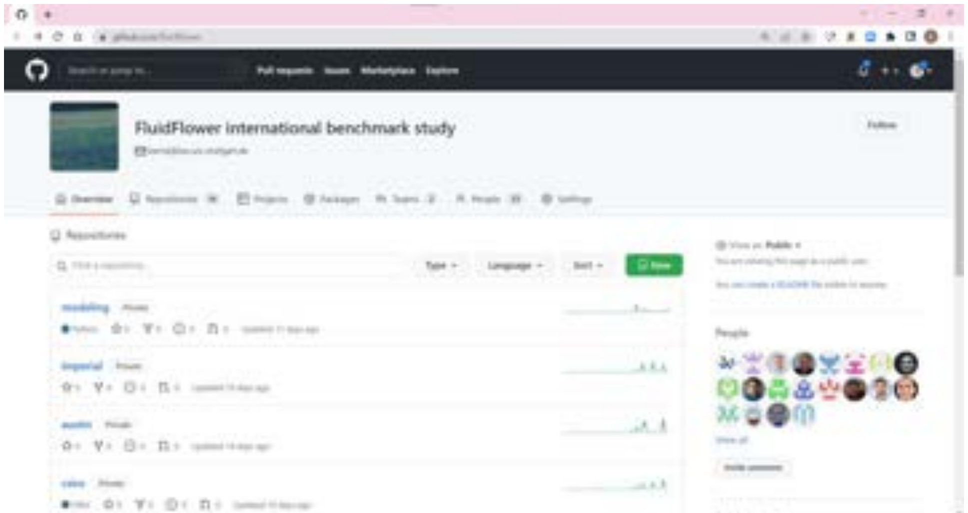
FluidFlower International Benchmark Study (2023)

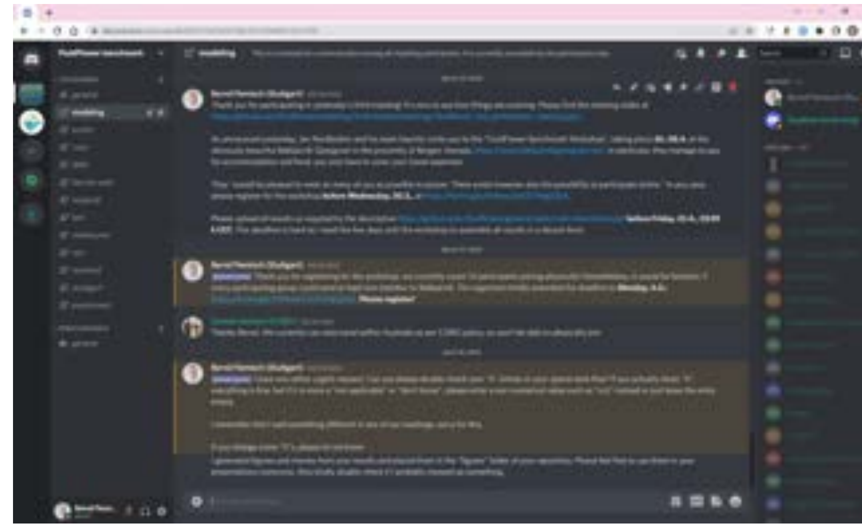
SRQs, Measures and Metrics

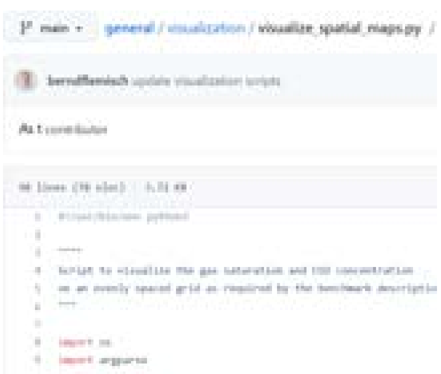


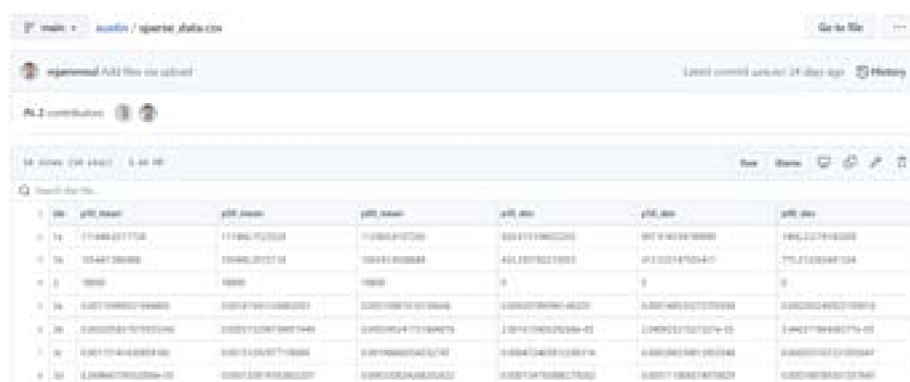
FluidFlower International Benchmark Study (2023)

Infrastructure for Comparison and Reproduction









Verification & Validation

Other Benchmark Studies

LH²

Comput Geosci (2009) 13:409–434
DOI 10.1007/s10596-009-9146-x

ORIGINAL PAPER

A benchmark study on problems related to CO_2 storage in geologic formations

Summary and discussion of the results

Holger Class · Anozie Ebigbo · Rainer Helmig · Helge K. Dahle ·
Jan M. Nordbotten · Michael A. Celia · Pascal Audigane · Melanie D
Jonathan Ennis-King · Yaqing Fan · Bernd Flemisch · S
Min Jin · Stefanie Krug · Diane Labregere · Ali N
Adil Sbai · Sunil G. Thomas · Laurent Tre

International Journal of Greenhouse Gas Control 9 (2012) 234–242

ELSEVIER

Contents lists available at SciVerse ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

...lation of CO_2 storage

... Y. Fan, G.E. Pickup, B. Wiese, M.A. Celia,

Upcoming: 11th SPE Comparative Solution Project

ELSEVIER

Adv...

journal homepage: www.elsevier.com/...

Benchmarks for single-phase flow in fractured porous media

Bernd Flemisch[a,*], Inga Berre[b], Wietse Boon[b], Alessio Fumagalli[b], Nicolas Schwenck[a], Anna Scotti[c], Ivar Stefansson[b], Alexandru Tatomir[d]

...020) 103759

... ScienceDirect

...s in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

Verification benchmarks for single-phase flow in three-dimensional fractured porous media

Inga Berre[a], Wietse M. Boon[b], Bernd Flemisch[c,*], Alessio Fumagalli[a,d], Dennis Gläser[c], Eirik Keilegavlen[a], Anna Scotti[d], Ivar Stefansson[a], Alexandru Tatomir[e,f], Konstantin Brenner[g], Samuel Burbulla[h], Philippe Devloo[i], Omar Duran[i], Marco Favino[j], Julian Hennicker[k], I-Hsien Lee[l,m], Konstantin Lipnikov[n], Roland Masson[g], Klaus Mosthaf[o], Maria Giuseppina Chiara Nestola[p], Chuen-Fa Ni[l,m], Kirill Nikitin[q], Philipp Schädle[r], Daniil Svyatskiy[n], Ruslan Yanbarisov[q], Patrick Zulian[p]

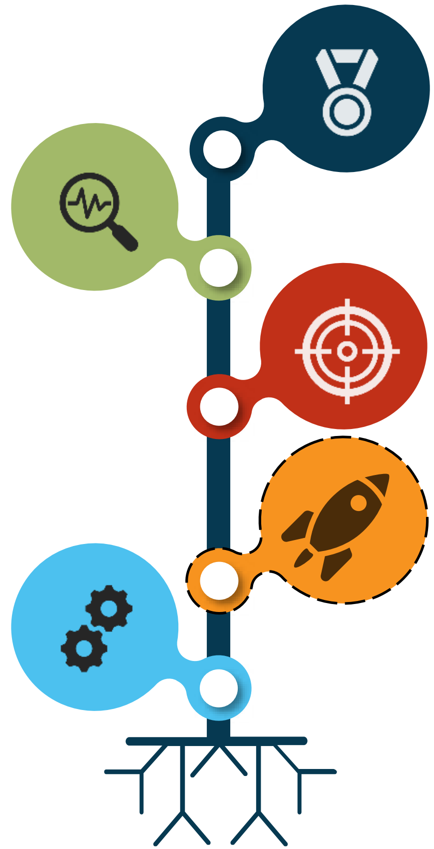
A Bayesian Validation Framework

Bayesian validation

- Uncertainty propagation using posterior
- Comparison with new data
- Computation of validation metric

Prior knowledge

- Input parameters
- Expert knowledge
- Computational Model(s)



Valid or not?

- Qualitative (visual) comparison
- Quantitative comparison
- Hypothesis testing

Bayesian calibration

- Bayesian inference
- Comparison with observation data
- Update prior knowledge to obtain posterior

Surrogate modeling

- Uncertainty propagation
- Speed-up of the inference step
- A cheap-to-evaluate model

F. Mohammadi, S. Oladyshkin, E. Eggenweiler, B. Flemisch, I. Rybak, M. Schneider, K. Weishaupt (2023): “A Surrogate-Assisted Uncertainty-Aware Bayesian Validation Framework and its Application to Coupling Free Flow and Porous-Medium Flow“, *in review*.

Outline

Overview

Development

Quality Assurance

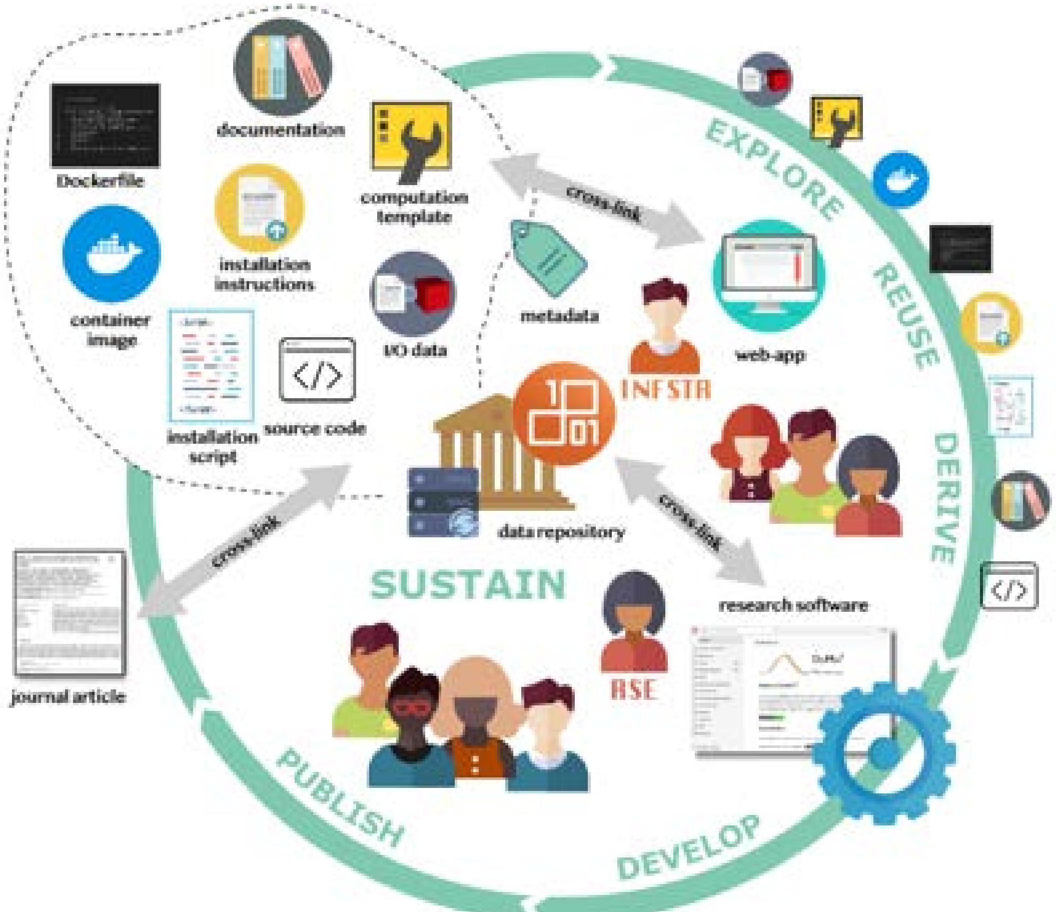
Verification & Validation

Reproducibility

Ingredients for Reproducing/Reusing Computations

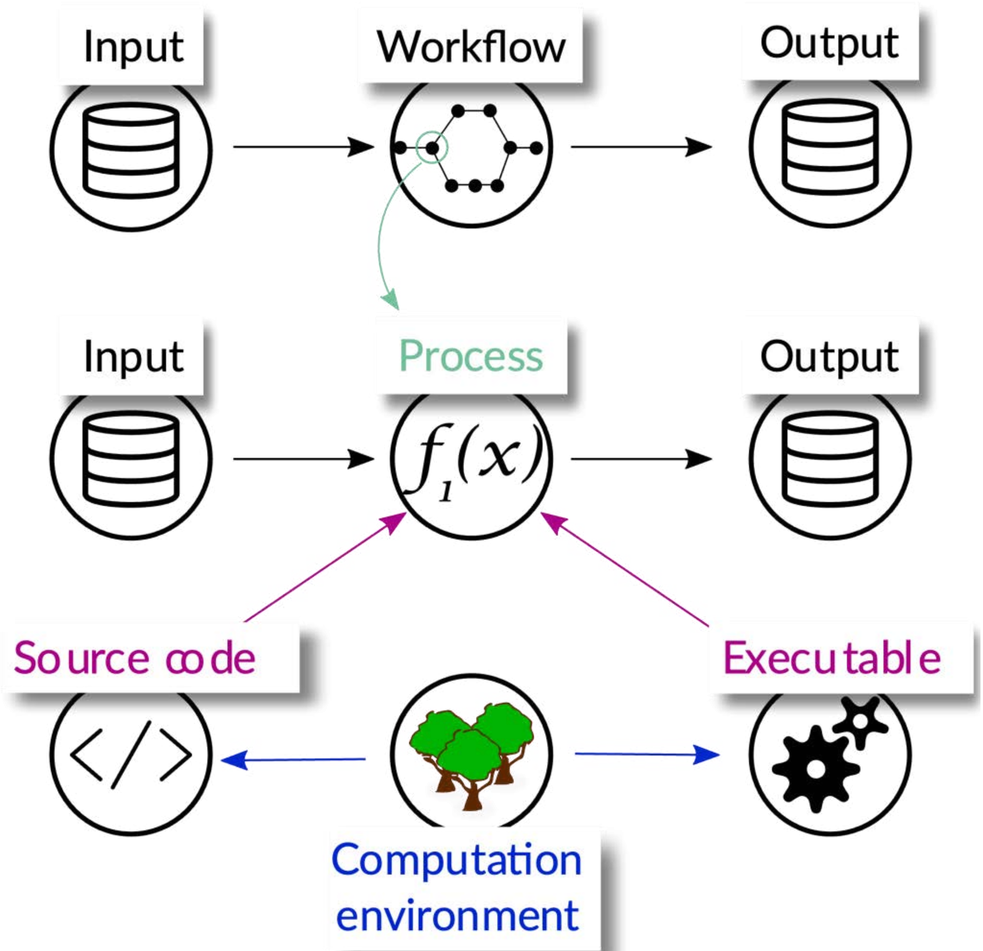
- FAIR research software
- Automation and Containerization
- Interactive reuse by browser-based-access
- Multi-modal software data repository

Improved accessibility, reusability, and archival of research software



T. Koch, D. Gläser, A. Seeland, S. Roy, K. Gönner, K. Weishaupt, D. Boehringer, S. Hermann, B. Flemisch (2023): “A sustainable infrastructure concept for improved accessibility, reusability, and archival of research software“, *in preparation*.

Digital Workflows



DEDUCTION OF REQUIREMENTS FOR

- REPRODUCIBLE
- REUSABLE
- EXTENSIBLE
- COMPOSABLE
- EFFICIENT
- …
- FAIR

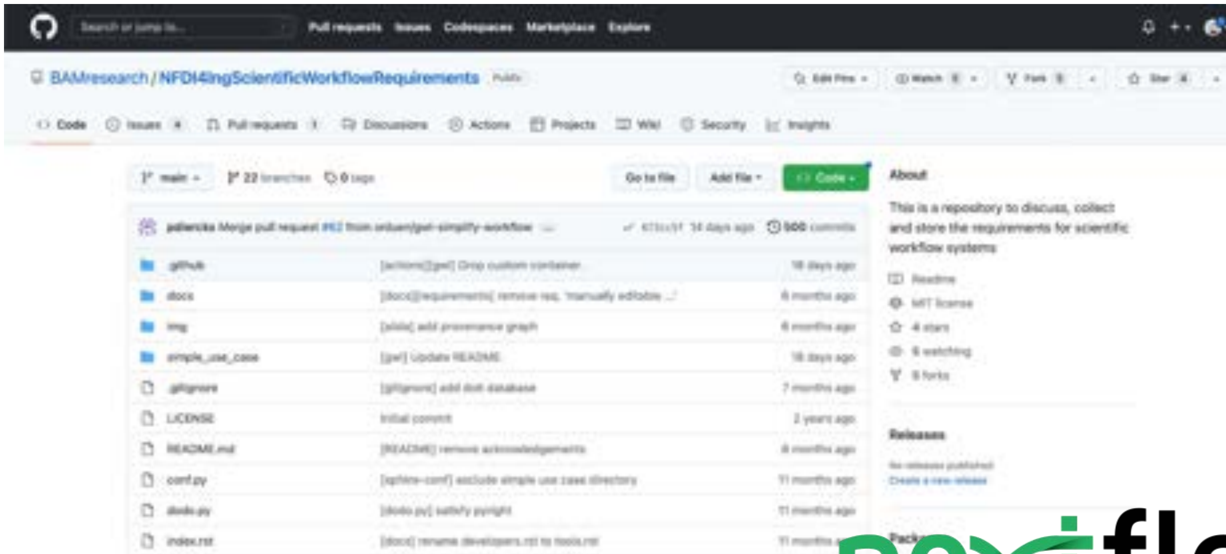
WORKFLOWS

Reproducibility

Workflow Tools: Implementations

NFDI4Ing

LH²



COMMON WORKFLOW LANGUAGE

DoIt Automation Tool

Kadi4Mat

nextflow

AiiDA

maestro

snakemake

github.com/BAMresearch/NFDI4IngScientificWorkflowRequirements

Workflow Tools: Manuscript

ing.grid preprints

RESEARCH ARTICLE

Evaluation of tools for describing, reproducing and reusing scientific workflows

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Dennis Gläser[2]
Ontje Lünsdorf[3]
Michael Selzer[4]
Bernd Flemisch[2]
Jörg F. Unger[1]

1. Department 7.7 Modeling and Simulation, Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin.
2. Lehrstuhl für Wasser- und Umweltsystemmodellierung, University of Stuttgart, Stuttgart.
3. Institut für Vernetzte Energiesysteme, Deutsches Zentrum für Luft- und Raumfahrt, Oldenburg.
4. Institut für Angewandte Materialien IAM, Karlsruher Institut für Technologie, Karlsruhe.

Date Received:
2022-12-05

Licenses:
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Keywords:
FAIR, reproducibility, scientific workflows, tool comparison, workflow management

Data availability:
Data can be found here:
https://github.com/BAMresearch/NFDI4IngScientificWorkflowRequirements

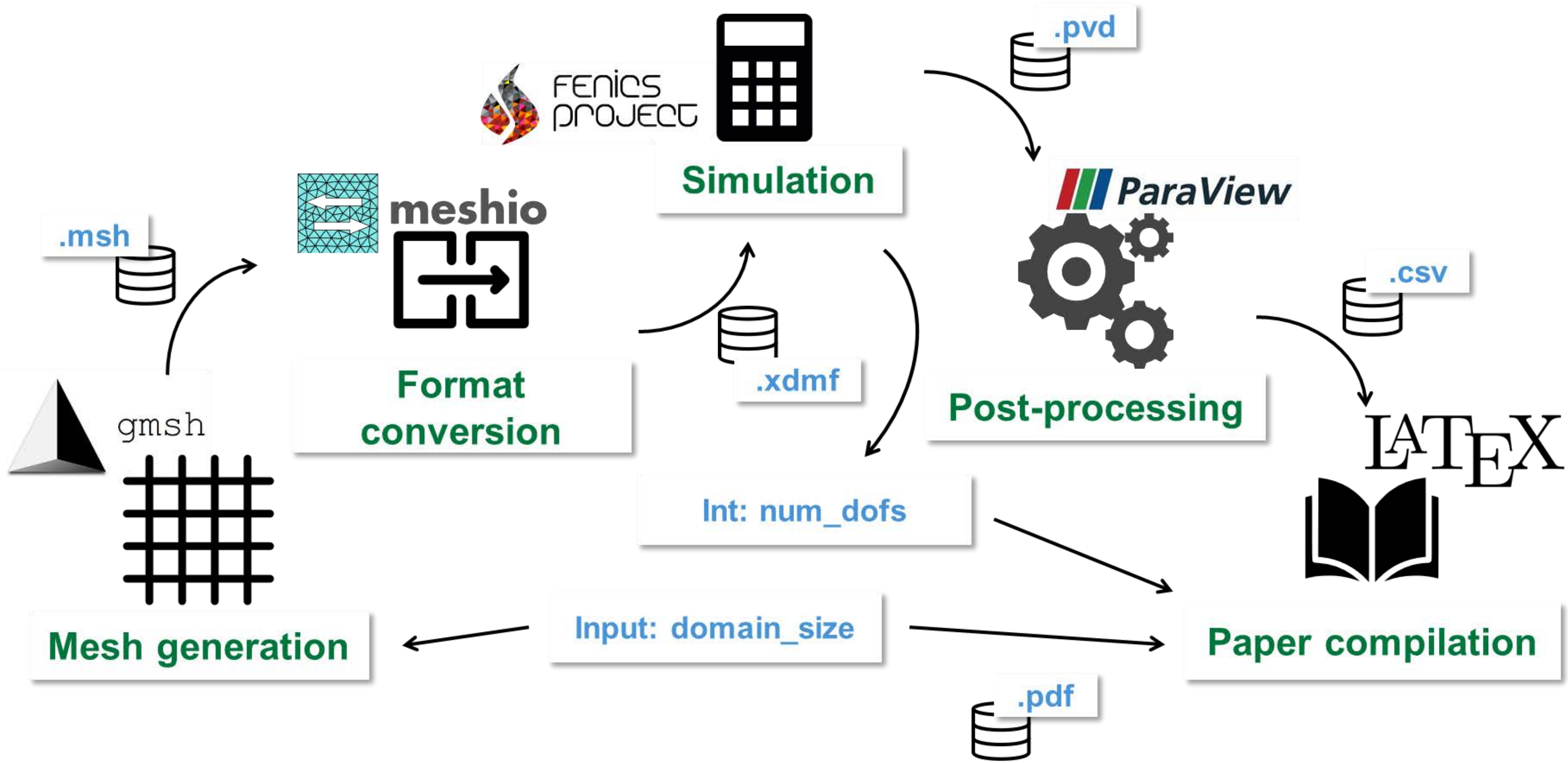
Software availability:
Software can be found here:
https://github.com/BAMresearch/NFDI4IngScientificWorkflowRequirements

Abstract. In the field of computational science and engineering, workflows often entail the application of various software, for instance, for simulation or pre- and postprocessing. Typically, these components have to be combined in arbitrarily complex workflows to address a specific research question. In order for peer researchers to understand, reproduce and (re)use the findings of a scientific publication, several challenges have to be addressed. For instance, the employed workflow has to be automated and information on all used software must be available for a reproduction of the results. Moreover, the results must be traceable and the workflow documented and readable to allow for external verification and greater trust. In this paper, existing workflow management systems (WfMSs) are discussed regarding their suitability for describing, reproducing and reusing scientific workflows. To this end, a set of general requirements for WfMSs were deduced from user stories that we deem relevant in the domain of computational science and engineering. On the basis of an exemplary workflow implementation, publicly hosted at GitHub (https://github.com/BAMresearch/NFDI4IngScientificWorkflowRequirements), a selection of different WfMSs is compared with respect to these requirements, to support fellow scientists in identifying the WfMSs that best suit their requirements.

1 Introduction

With increasing volume, complexity and creation speed of scholarly data, humans rely more and more on computational support in processing this data. The "FAIR guiding principles for scientific data management and stewardship" [41] were introduced in order to improve the ability

Workflow Tools: Simple Use Case



Summary

- **Development**
  - Standardized Git workflow enforced by GitLab policies or instructed
  - Release process is “standardized” via issue template
- **Quality Assurance**
  - Automated test pipelines for various setups
  - Mainly regression testing of small simulations
- **Verification & Validation**
  - Benchmarking allows model evaluation and comparison
  - Uncertainties in models and experiment should be quantified
- **Reproducibility**
  - Key ingredients are automation and containerization
  - Possibly facilitated by workflow tools

Is DuMu^x right for you?

- Large **variety** of available models.
- Flexible monolithic **coupling** framework.
- Focus on **model development** rather than applications (or numerics).
- **Not** a “classical” reservoir simulator.
- “Easy” to customize/add **balance equations** and **constitutive relations.**
- Adding new **discretization methods** is challenging.
- **C++** skills are required to do something substantially new.
- **Python** bindings are working, but not fully exploited yet.
- Friendly and welcoming **user/developer community.**

- **Find out at this year’s DuMu^x course 3.-5.4.2023 in Stuttgart:**

University of Stuttgart
Germany

Thank you!

Bernd Flemisch

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phone +49 (0) 711 685- 69162

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Department of Hydromechanics and Modelling of Hydrosystems
Pfaffenwaldring 61, 70569 Stuttgart, Germany