EURAD2 - HERMES

Task 3: THMC-Process Couplings and Computational Performance

Task lead:
Anne-Catherine Dieudonné / Olaf Kolditz

Agenda

- Lessons learned from EURAD1 (Claret et al. 2024)
- Modelling strategy
  - Automated workflows (data integration, benchmarking, site modeling)
  - Computational efficiency (HPC)
  - Machine Learning
  - …
- Model-Hub
- Highlights
- Synthesis


frontiers | Frontiers in Nuclear Engineering

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EURAD state-of-the-art report: development and improvement of numerical methods and tools for modeling coupled processes in the field of nuclear waste disposal

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The Strategic Research Agenda (SRA; https://www.ejp-eurad.eu/publications/eurad-sra) of the European Joint Programme on Radioactive Waste Management (EURAD; https://www.ejp-eurad.eu/) describes the scientific and technical domains and sub-domains and knowledge management needs of common interest between EURAD participant organizations. Theme number 7 is entitled "Performance assessment, safety case development and safety analyses." A list of research and development priorities and activities of common interest to be addressed within EURAD for theme 7 have been

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Introduction

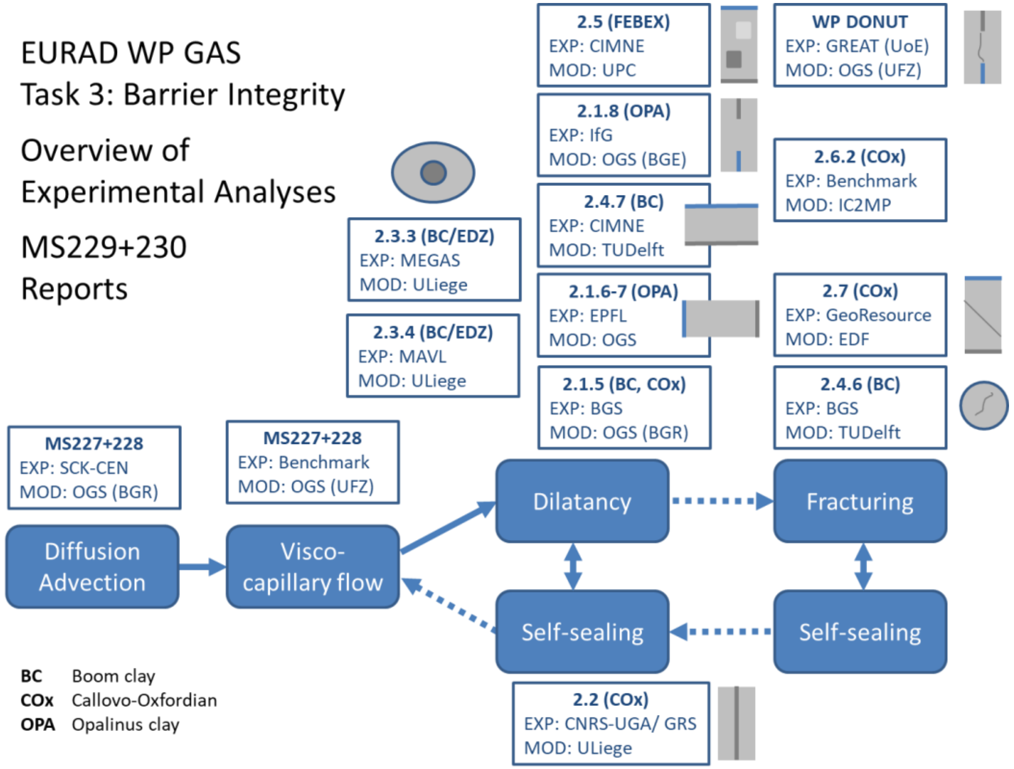
EURAD-1: Review: GAS (H2M / TH2M)

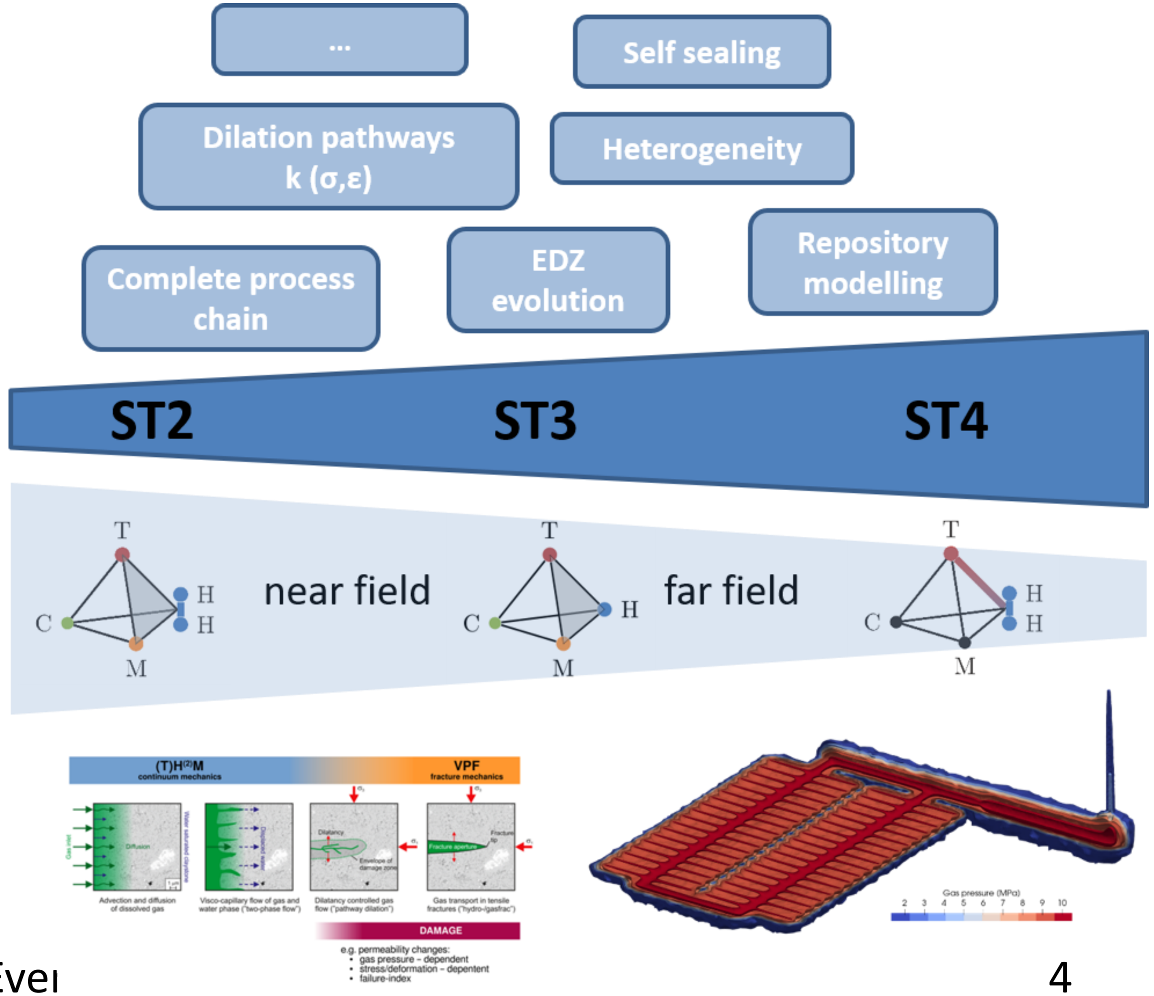
Implementation >>> Synthesis

EURAD WP GAS
Task 3: Barrier Integrity

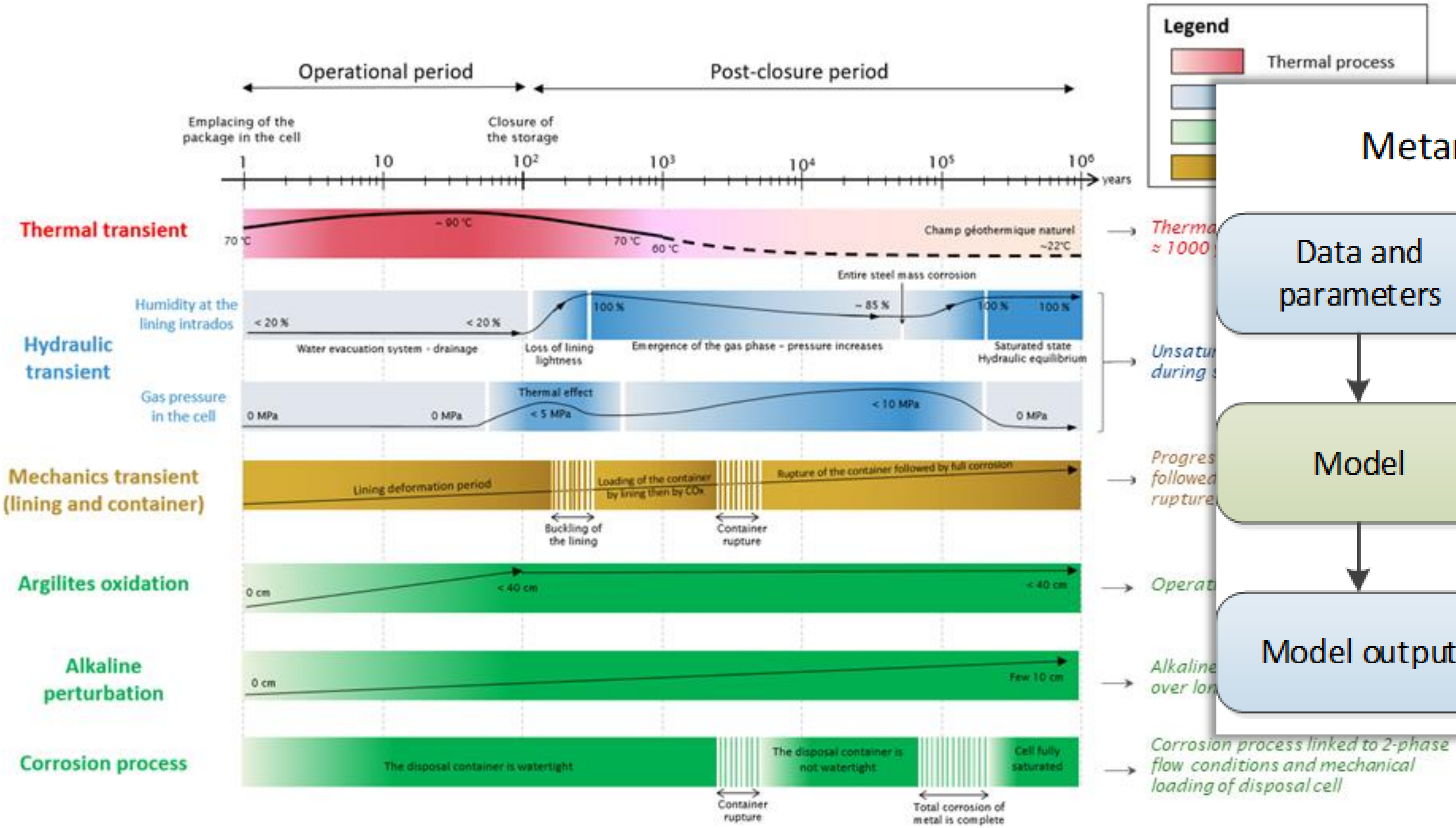
Overview of
Experimental Analyses

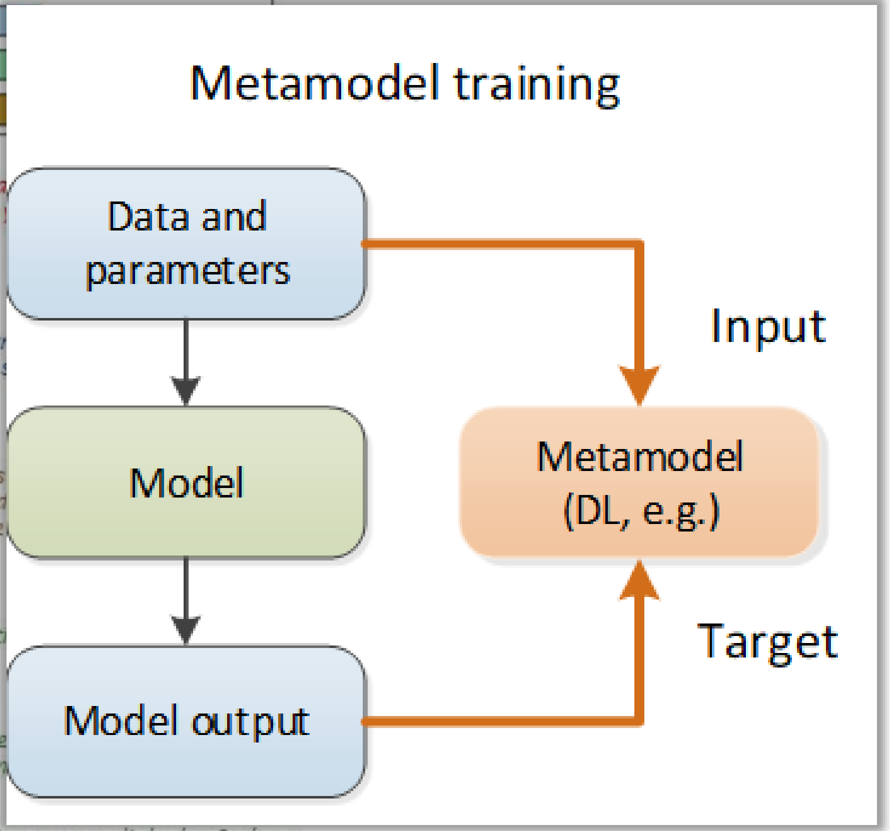
MS229+230
Reports





THMC processes





Churakov et al. 2024
Claret et al. 2024

Workflows >> DTw

Environmental Earth Sciences (2023) 82:42
https://doi.org/10.1007/s12665-022-10675-4

EDITORIAL

Digitalisation for nuclear waste management: predisposal and disposal

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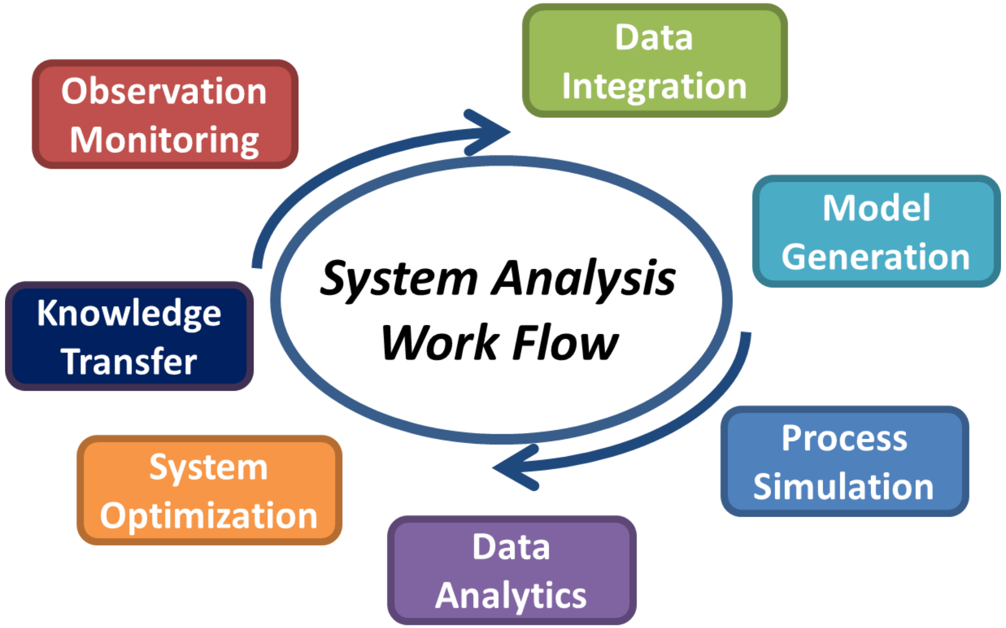
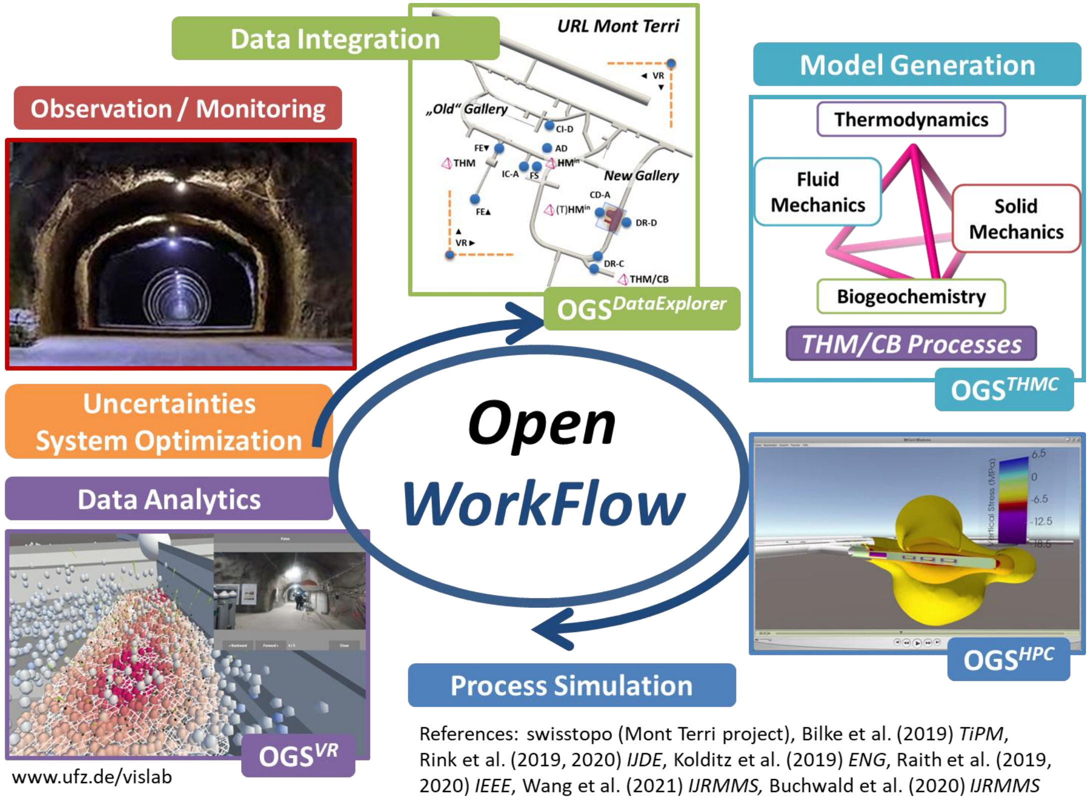


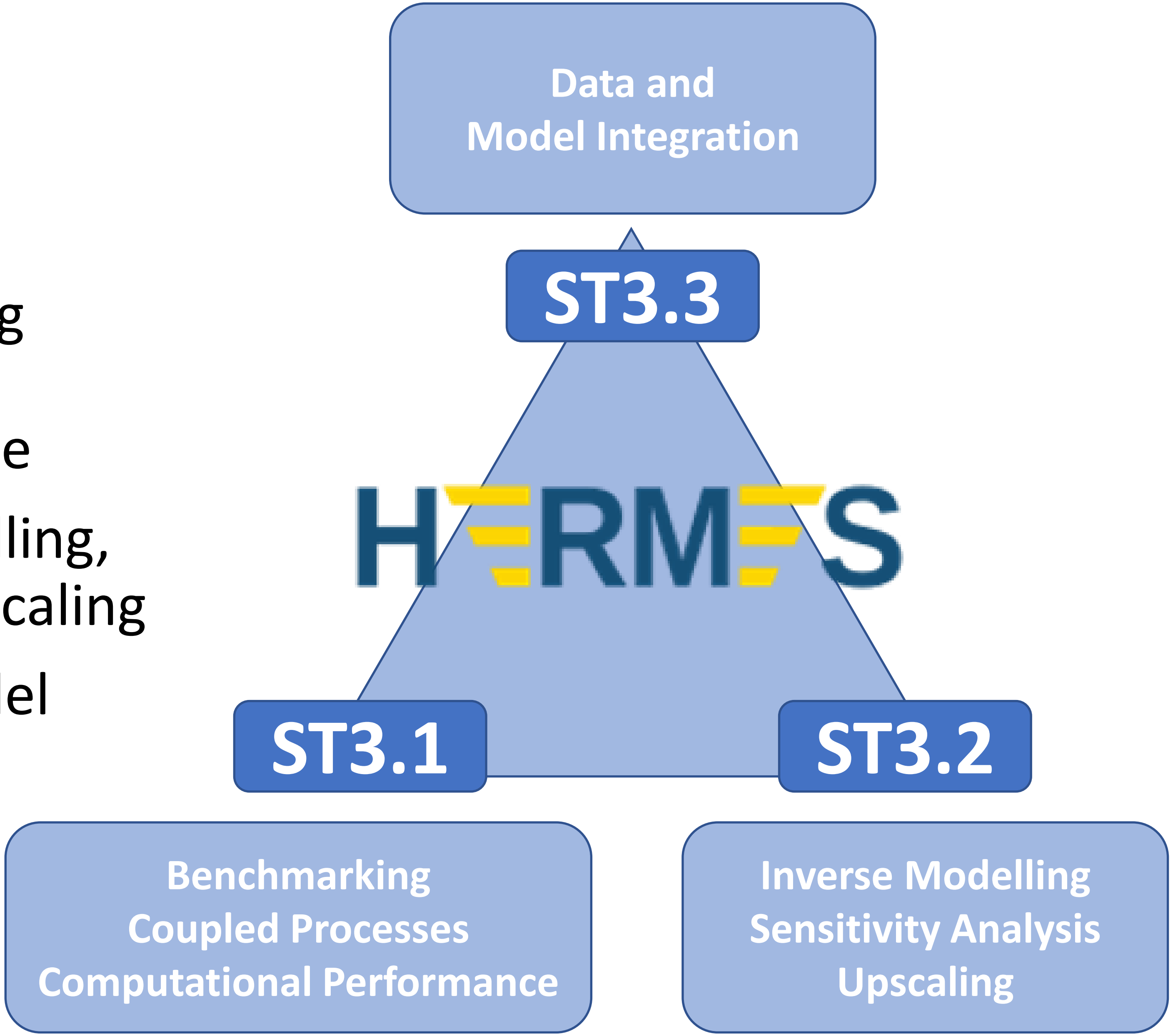


References: swisstopo (Mont Terri project), Bilke et al. (2019) *TiPM*, Rink et al. (2019, 2020) *IJDE*, Kolditz et al. (2019) *ENG*, Raith et al. (2019, 2020) *IEEE*, Wang et al. (2021) *IJRMMS*, Buchwald et al. (2020) *IJRMMS*

Task 3

Task 3: Structure

- SubTask 3.1: Benchmarking coupled processes and computational performance
- SubTask 3.2: Inverse modelling, sensitivity analysis and upscaling
- SubTask 3.3: Data and model integration



Task 3: Compact

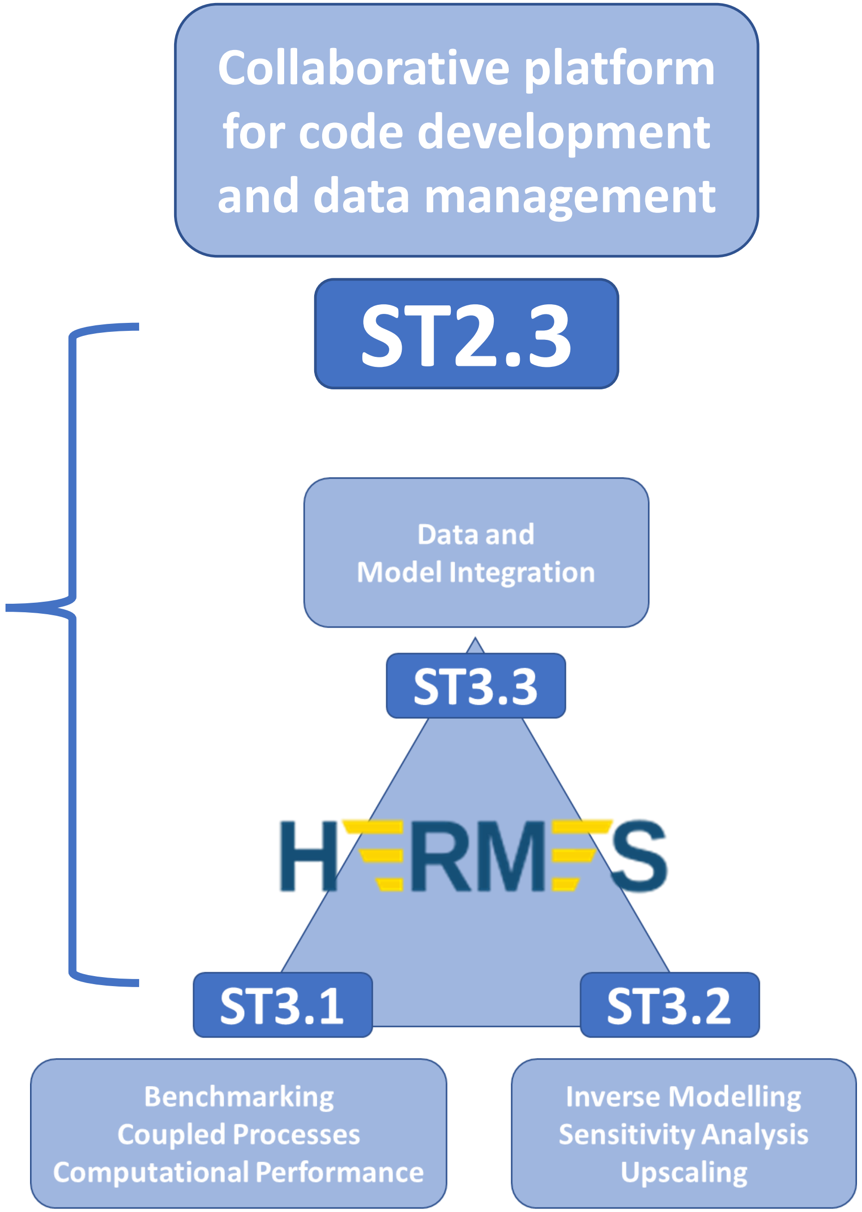
- SubTask 3.1: Benchmarking coupled processes and computational performance
  - coupled processes: Multiphysics + chemistry, L/ILW and HLW (combined repos)
  - numerical methods
  - computational performance (HPC)
- SubTask 3.2: Inverse modelling, sensitivity analysis and upscaling
  - sensitivity analyses (variety of methods)
  - inverse modelling (e.g. ROM)
- SubTask 3.3: Data and model integration

Task 3: Integration

- SubTask 3.3: Data and model integration

###

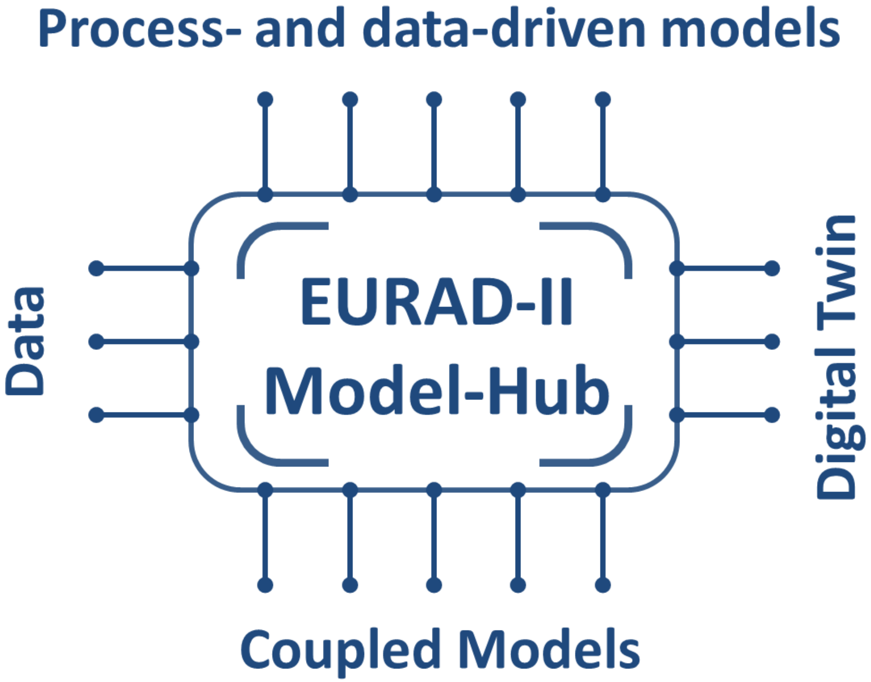
- SubTask 2.3: Collaborative platform for code development and data management



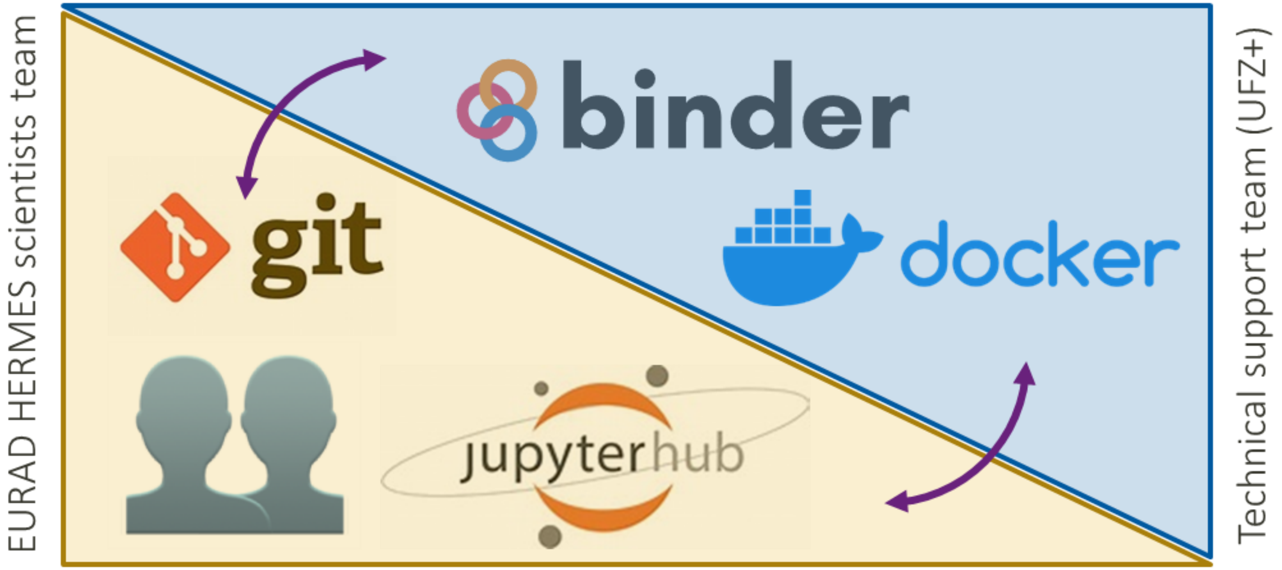
Model Hub

Collaborative platform for code development and data management

Concept >>> Implementation

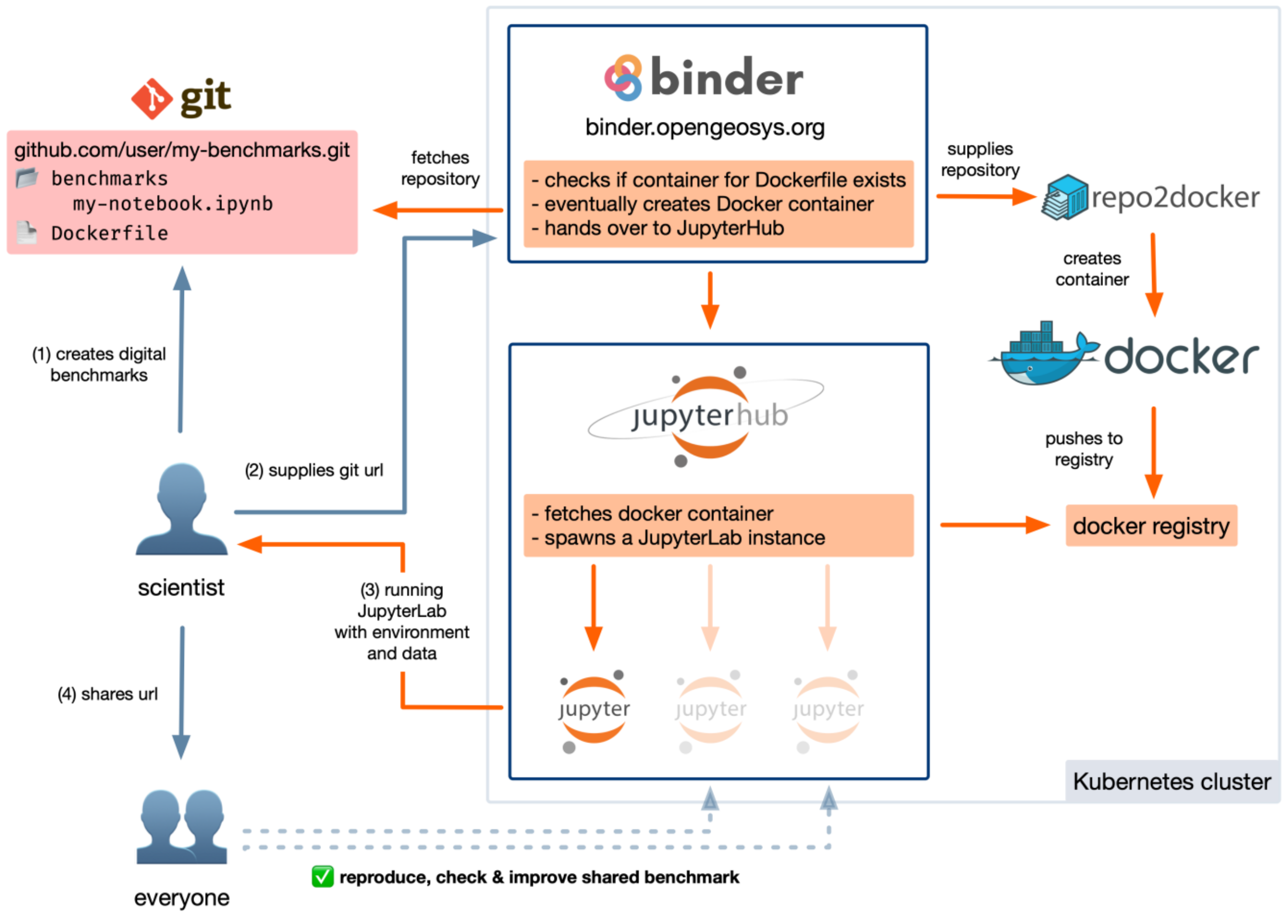


binder: providing the computational web-platform
docker: providing the software environment (Python et al.)



git: version-management for repos (scientists + hermes)
jupyterhub: working environment for scientists

Collaborative platform for code development and data management

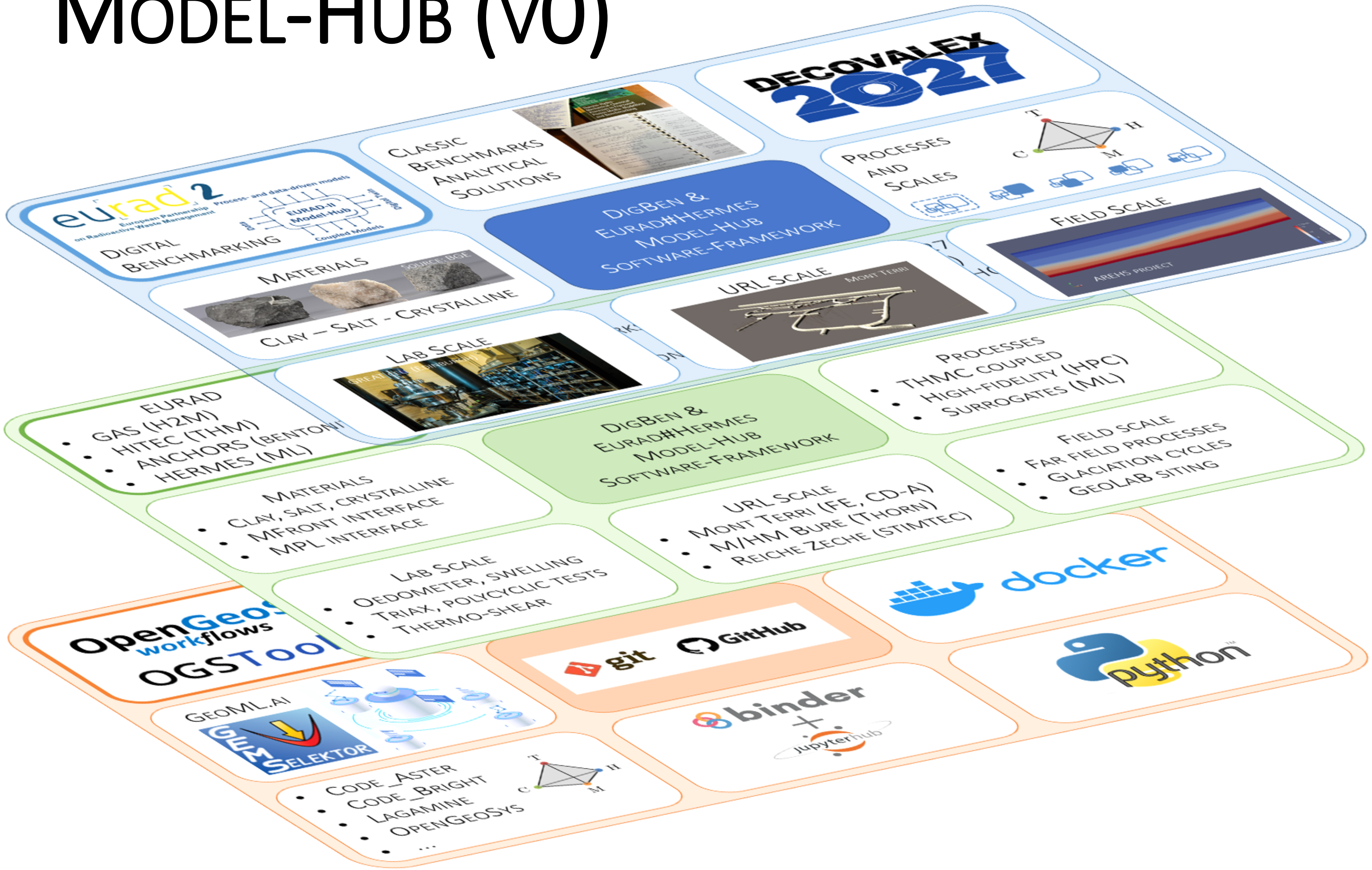


Technical layout and implementation

- Admin side (UFZ)
  - Hardware#Software (UFZ server)
  - github # jupyterhub # binder # docker
- Users side
  - writing **jupyter notebooks** for benchmarks (and later applications)
  - UFZ/TUBAF will provide templates
  - local testing on users side
  - pushing to hermes github (**git**)
- Part of the DigBen project (+BGR)

European Partnership on Radioactive Waste Management

Model-Hub (v0)



WebLayer

structured user-web-interface organized by thematic areas: materials, processes, scales > projects

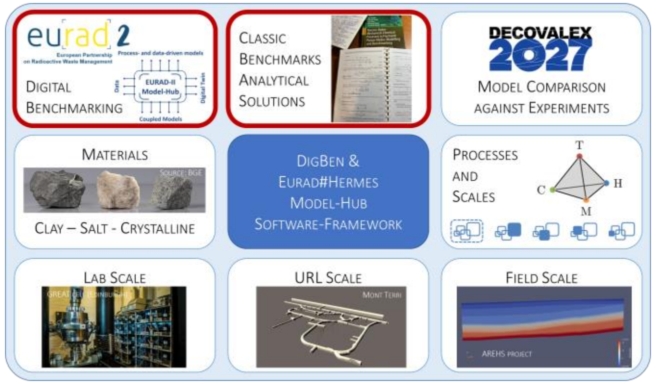
InfoLayer

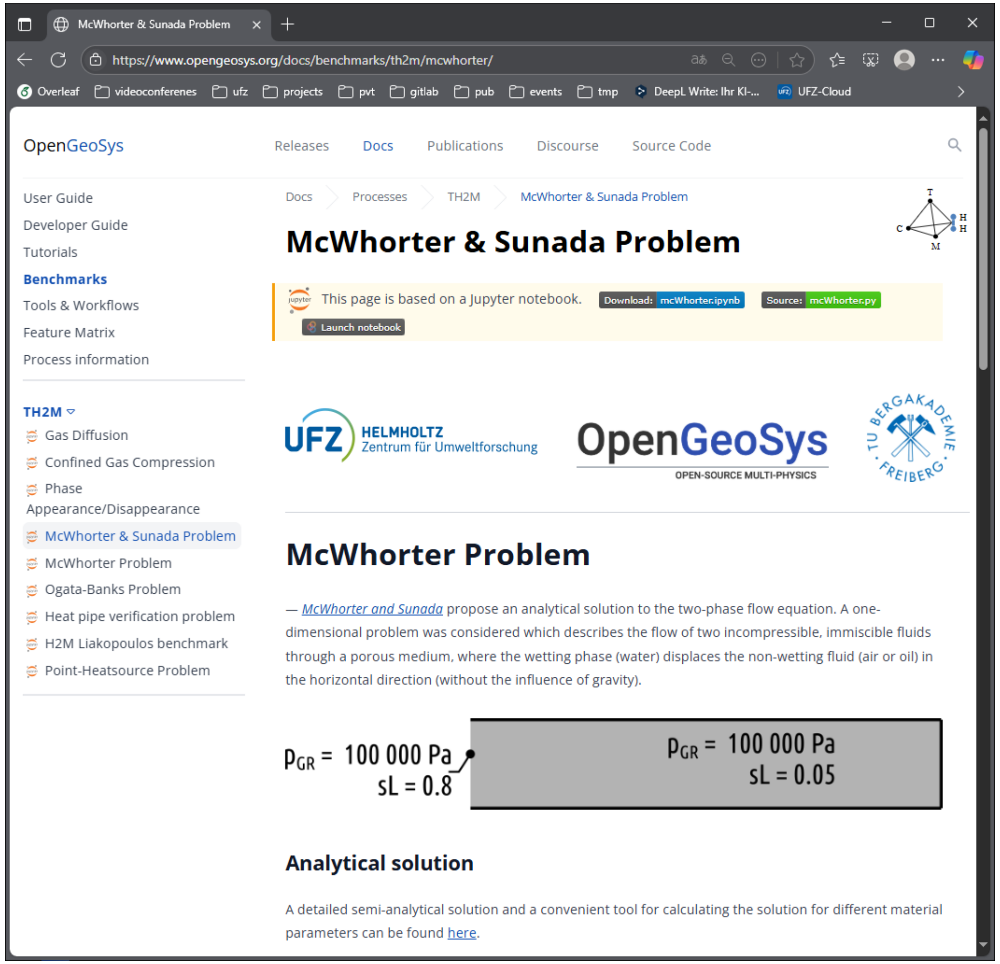
specific information about thematic areas including literature links > list of current benchmarks and examples (extending)

JupyterLab

interactive Jupyter Notebooks of benchmarks and examples < coding area for interactive work

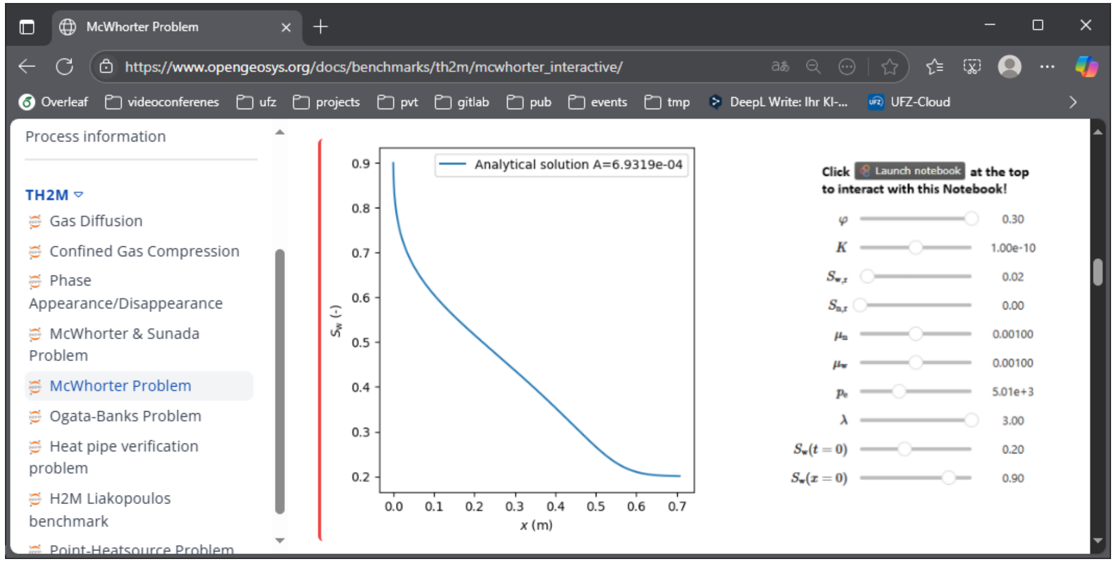
Model-Hub: Classic Benchmarks



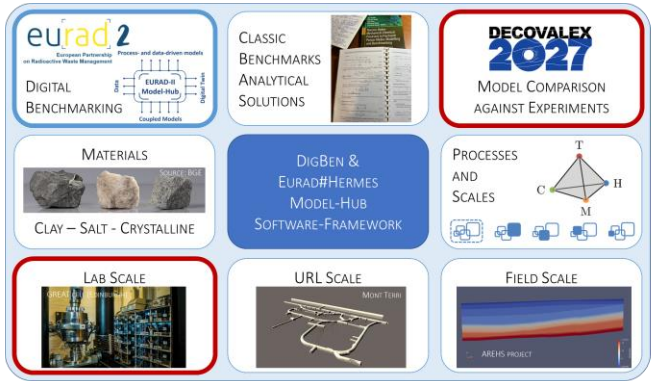


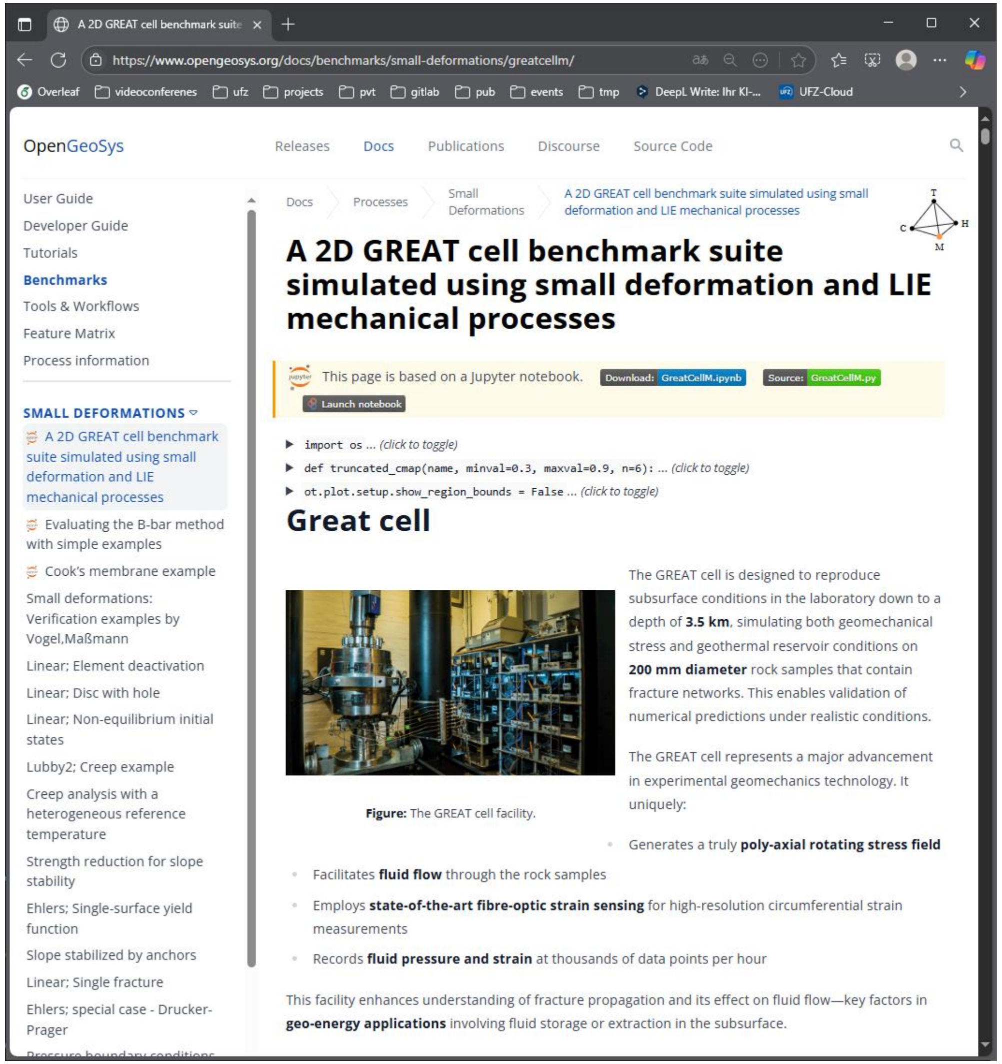
[McWhorter Problem](https://www.opengeosys.org/docs/benchmarks/th2m/mcwhorter/)

- Two-phase flow in porous media
- Analytical solution as benchmark test for numerical models
- Interactive Jupyter notebook (two-phase flow parameters)



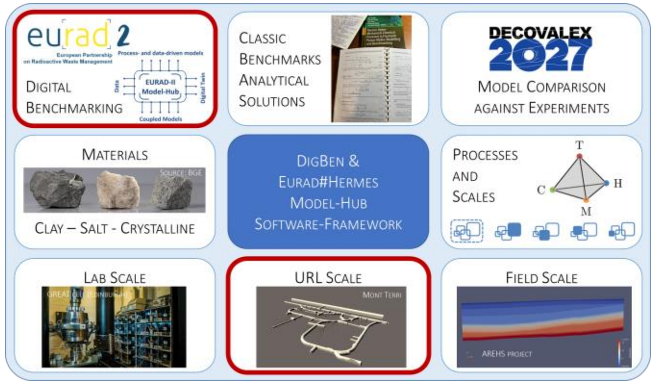
Model-Hub: Lab Scale



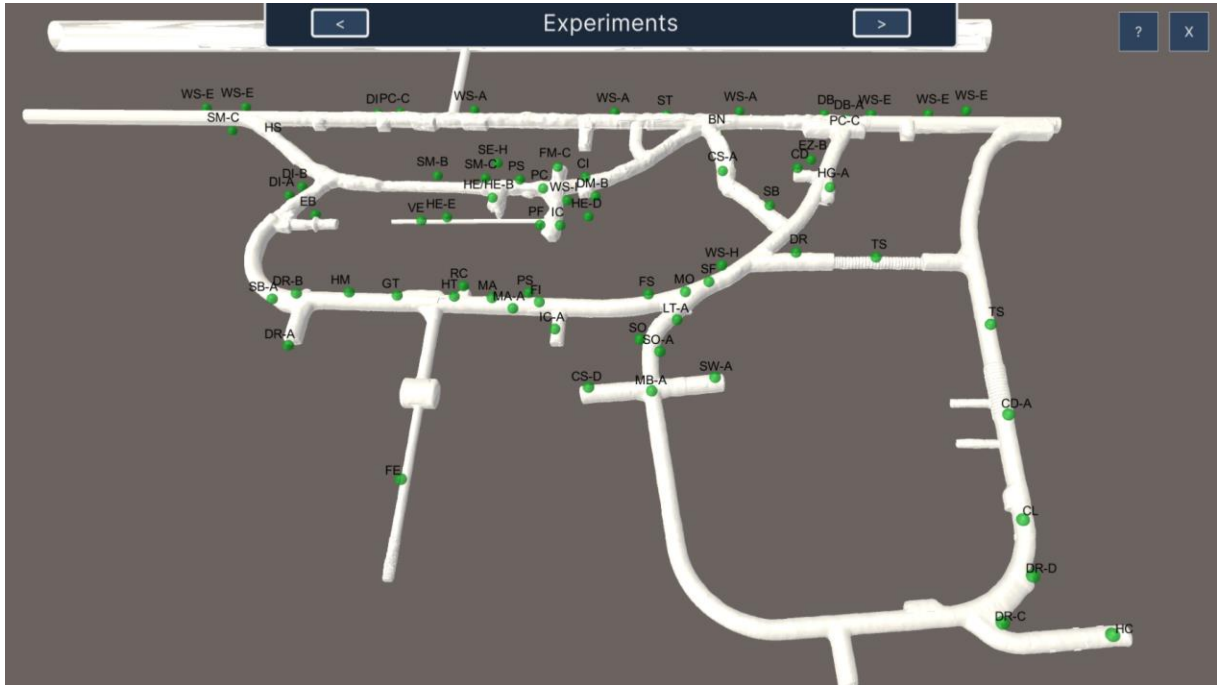


- Link to the DECOVALEX projects
- GREAT cell experiments: polyaxial cell for THM processes (Uni Edinburgh)
- Strength of crystalline rocks during stress orientation changes
- Fracture nucleation and propagation
- Comparison of various numerical methods for fracture mechanics
- Development of an experimental based, comprehensive benchmark suite

[A 2D GREAT cell benchmark suite simulated using small deformation and LIE mechanical processes]



Model-Hub: URL Scale



https://www.opengeosys.org/docs/benchmarks/reactive-transport/co2injection/

https://www.opengeosys.org/docs/benchmarks/reactive-transport/radionuclidesmigration/

Current experiment models inURL Mont Terri

- Full Explacement (FE) > minibenchmarks
- Cyclic Deformation (CD-A)
- Fault Slip (SP)

Reactive Transport Processes

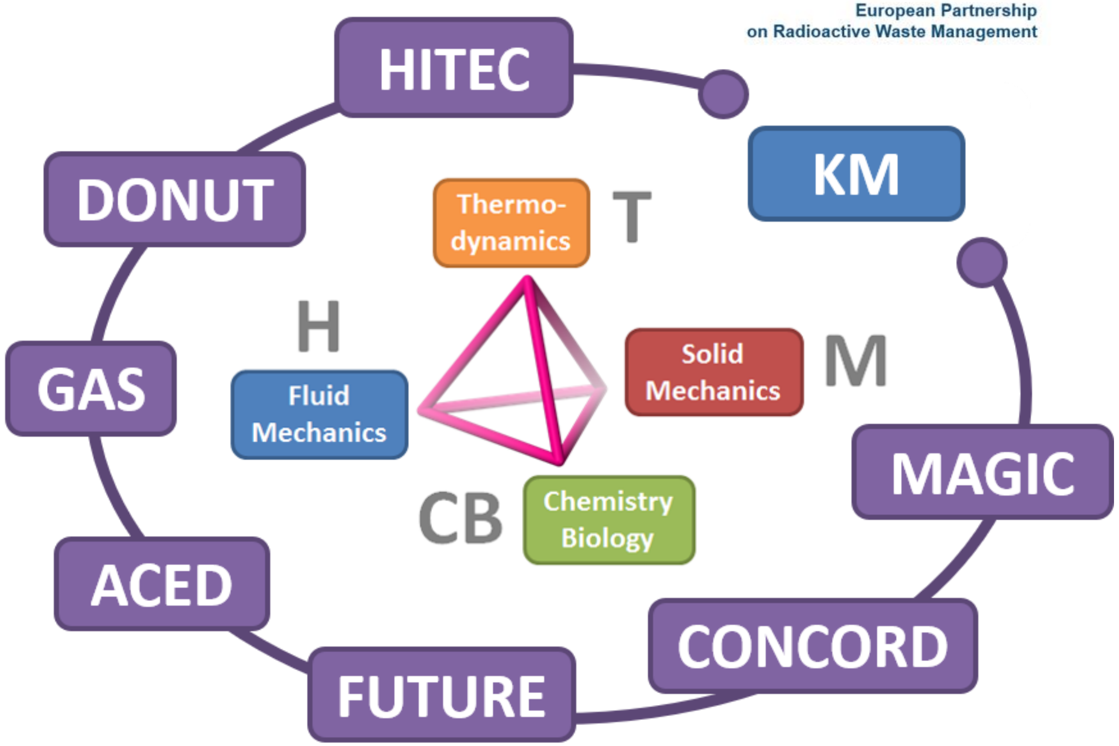
- Non-isothermal Diffusion (DR-D)
- CO2 Injection into OPA (CL)
- Radionuclide migration (CI)

Highlights

Highlights - Examples

Networking & Synthesis

EURAD-2: Networking / Build-on THMC modelling



Environmental Earth Sciences (2024) 83:521
https://doi.org/10.1007/s12665-024-11832-7

ORIGINAL ARTICLE

Position paper on high fidelity simulations for coupled processes, multi-physics and chemistry in geological disposal of nuclear waste

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Abstract

This opinion paper describes the major coupled T(Thermal)-H(Hydro)-M(Mechanical)-C(Chemical) processes in geological repository systems and the frontier of related model development. Particular focus is made on the analysis of existing approaches and open research questions with respect to the further development of coupled codes and models for realistic multi-scale simulations of repository systems. These include the use of machine learning and artificial intelligence in acceleration of computer codes; sensitivity analysis, inverse modelling and optimisation; software engineering and collaborative platforms for model development.

Keywords T-H-M-C processes · Reactive transport · High fidelity simulations · Surrogate models

Introduction

Safe geological disposal of radioactive waste relies on a combination of engineered and natural barriers representing a so called multiple barrier approach (Apted and Ahn 2017). Natural barriers, e.g., the host rocks, are chosen to provide stable hydro-chemical-geo-tectonic conditions and to slow-down a potential migration of radionuclides into the biosphere. Depending on the thermo-hydro-chemo-mechanical conditions provided by the host rocks, the system of engineered barriers containing the waste is optimised to ensure the mechanical integrity of waste packages, and to delay possible release of soluble radionuclides into the host rocks and biosphere (IAEA 2020).

The whats and whys of repository systems and coupled processes

Based on its physical-chemical properties and radiotoxicity, radioactive waste is grouped into Spent (nuclear) Fuel/High Level Waste (SF/HLW) and Low-/Intermediate Level Waste (L/ILW) (IAEA 2009). Accordingly, different concepts are used for the design of the either waste repository types.

The SF/HLW is also referred to as heat emitting waste. Depending on the inventory of spallation products and the predisposal history of the SF, its thermal output can have significant implications for the time evolution of the thermo-hydro-chemo-mechanical conditions in the repository. The combination of thermal pulse, mechanical strain, pore pressure build-up, solutes and moisture transport leads to complex transient conditions (Seyedi et al. 2017). These processes are coupled to chemical gradients and heterogeneous reaction fronts evolving in the engineered barrier system (EBS) and even in the adjacent host rocks (Bildstein et al., 2019b; Leupin et al. 2016a).

L/ILW is typically immobilised by using a cement based matrix (Ojovan et al. 2019). Other binders such as bitumen and geopolymers have also been used or are being considered. Cementitious materials are known for their durability, schielding capability, mechanical performance and

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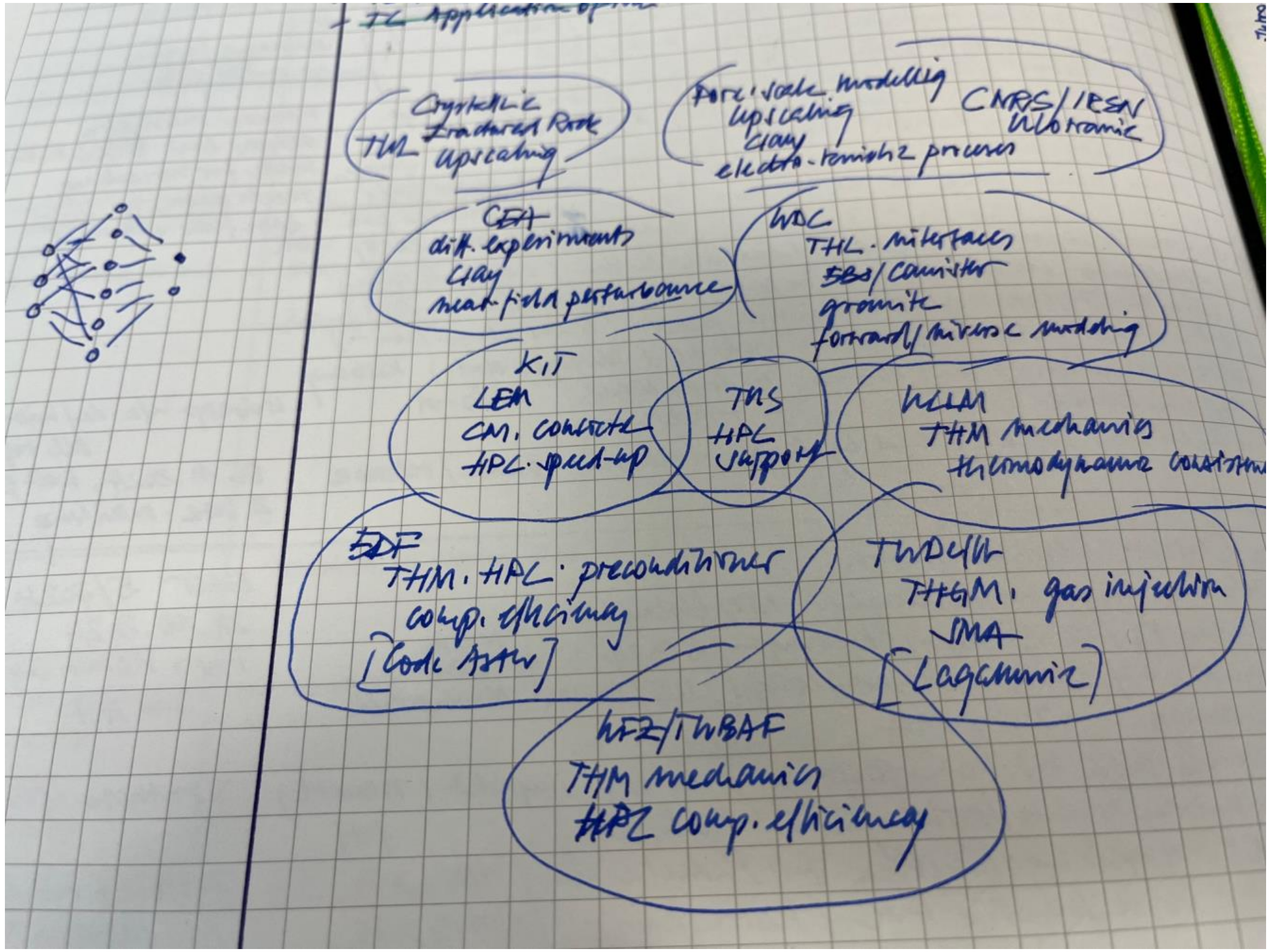
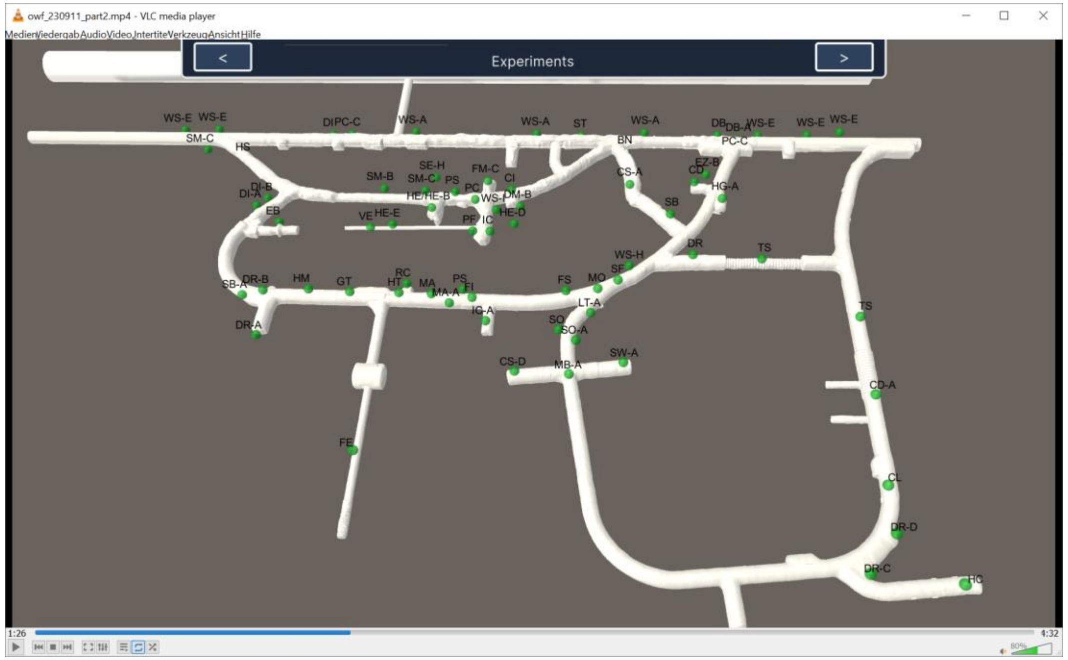
Springer

Collaborative platform for code development and data management

- Collaboration maps
  - within Tasks
  - beyond Tasks
  - beyond WPs



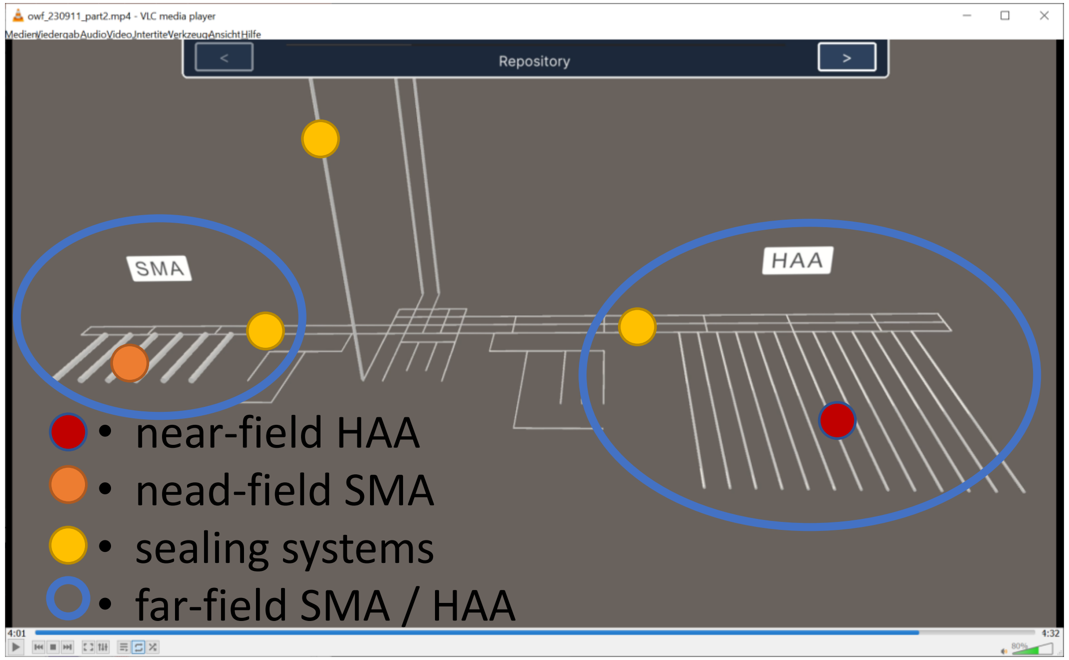
Collaborative platform for code development and data management



Mont Terri (Digital Twin)

„Repo-Concept“ (model repositories)

linking models (and data) to repository modules ...



Back-up area