European Partnership on Radioactive Waste Management

EURAD2 Annual Event 2025

Digital Transformation

DITICO2o3o and HERMES

Model-Hub

Bologna – 09-11.09.2025

Co-funded by the European Union under Grant Agreement n° 101166718

Agenda

HERMES Model-Hub

Preface

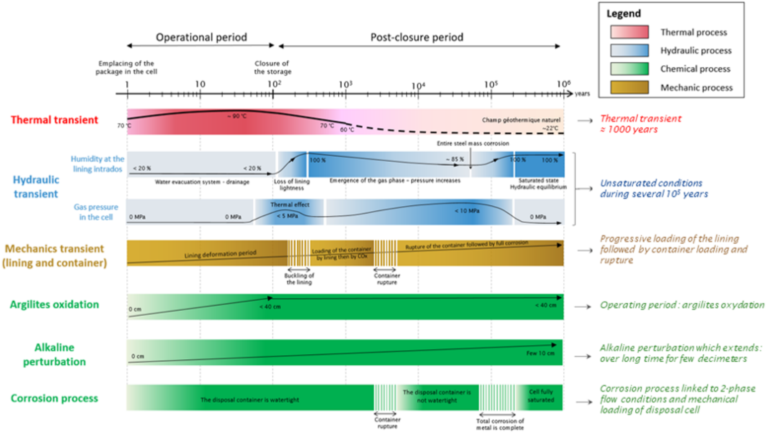
- Lessons learned from EURAD1 [4]
- Opinion Papers [6, 3]
- ↦ Modelling strategy for EURAD2
  - **Automated workflows** (data and model integration)
  - Computational efficiency (HPC)
  - Machine Learning (Task 4)
- **Model-Hub**

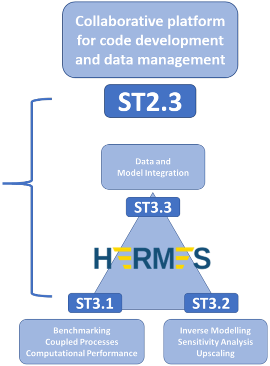
Top 1

Introduction

THMC Processes

EURAD HERMES Task 3





Churakov et al. (2024) Position paper on THMC processes and modeling [3]

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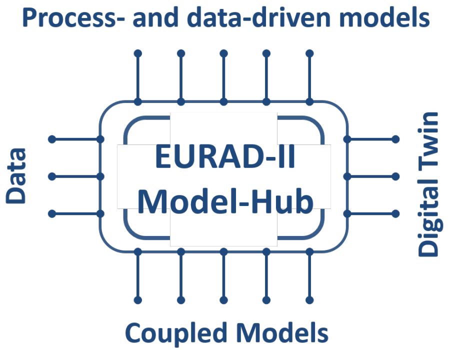
Model-Hub

Collaborative platform for data and model integration

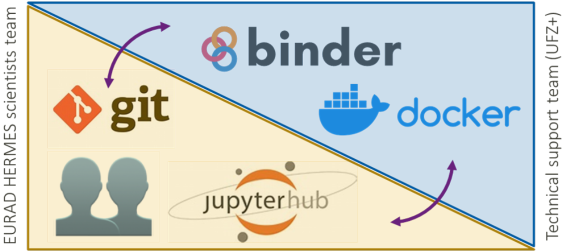
Model-Hub (HERMES Kick-Off (11/2024)

Idea



Implementation concept

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

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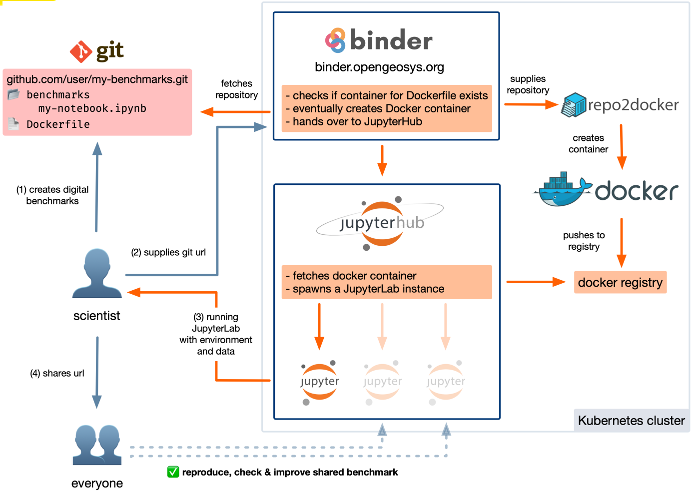
Collaborative platform for data and model integration

Model-Hub: Infrastructure development (available 09/2025)



Admin side (UFZ server)

- hard- and software
- OGSTools
- container technology
- git version management

User side

- interesting examples
- Jupyter notebooks
- GitLab skills

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Collaborative platform for data and model integration

Model-Hub: Thematic Web-Interface (available 09/2025)

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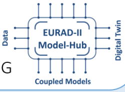
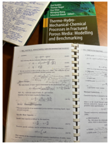
Process- and data-driven models



DIGITAL BENCHMARKING

CLASSIC BENCHMARKS
ANALYTICAL SOLUTIONS



DECOVALEX 2027

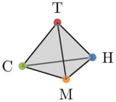
MODEL COMPARISON AGAINST EXPERIMENTS

MATERIALS

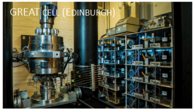
CLAY – SALT - CRYSTALLINE

DIGBEN &
EURAD#HERMES
MODEL-HUB
SOFTWARE-FRAMEWORK

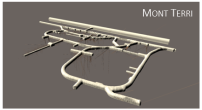
PROCESSES AND SCALES



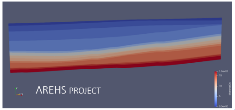
LAB SCALE



URL SCALE



FIELD SCALE



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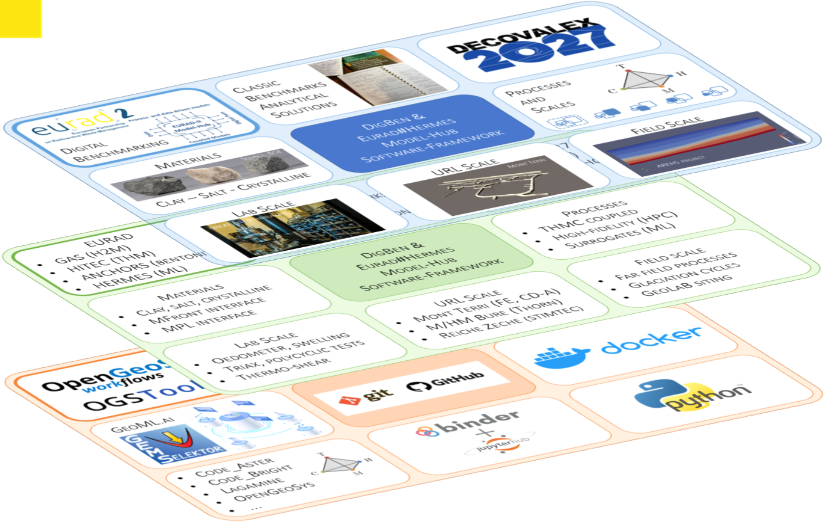
Collaborative platform for data and model integration

Model-Hub: Layer-Structure



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

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Model-Hub Demo

https://www.opengeosys.org/hub/

Top 4

Synthesis and Next

Synthesis

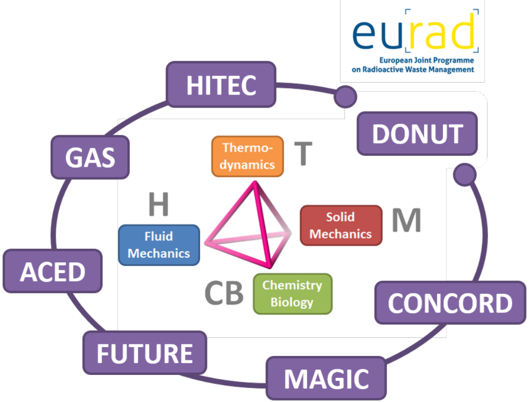
added value

What added value does the Model Hub bring?

- fosters networking on strategic AND technical levels, Claret et al. (2024) [4]
- contribution to KM
- contribution to FAIR

Workflows and Automation are prerequisites for Digital Twins (DITOCO)

EURAD Digi-Session on safeND 2025 (next week in Berlin)



Next ↦

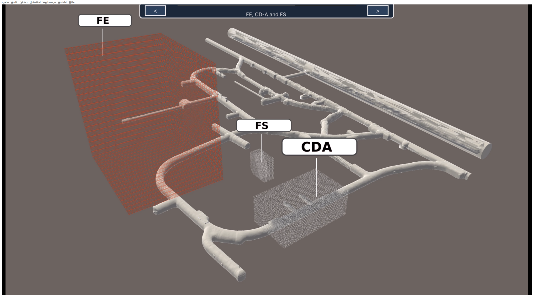
With Jupyter Notebooks (ipynb) to Workflows (snakemake/aiida)

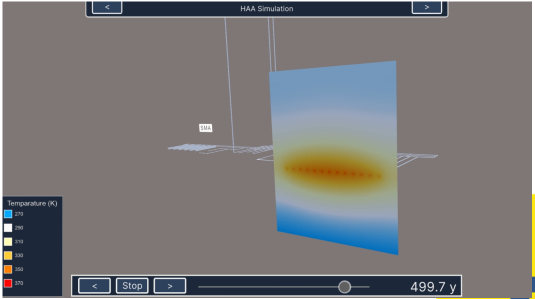
Benchmarking

- ANCHORS benchmarking exercises
- HERMES Annual Meeting (24-25.11.2025 Leipzig) hackathon for integration
- DECOVALEX links

Workflows for complex applications

- ipynb's can be fully integrated (e.g. tools for performance/safety indicators)
- Data and model integration in Mont Terri, Graebling et al. (2024) [5]
- Workflows for safety cases (snakemake, aiida), Bilke et al. (2025) [1]





Acknowledgements and Partners

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DigBen OpenWorkFlow

Bundesministerium
für Bildung
und Forschung

BGE

UFZ BGR TU BERGAKADEMIE · FREIBERG ·

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[2] Jens T. Birkholzer et al. "DECOVALEX-2023: An international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems". In: Geomechanics for Energy and the Environment 42 (2025). Cited by: 0. DOI: 10.1016/j.gete.2025.100685. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-105006976962&doi=10.1016%2fj.gete.2025.100685&partnerID=40&md5=a79e864363093548fd3a6cf19bb5c941.

[3] S.V. Churakov et al. "Position paper on high fidelity simulations for coupled processes, multi-physics and chemistry in geological disposal of nuclear waste". In: Environmental Earth Sciences 83.17 (2024). Cited by: 4; All Open Access, Hybrid Gold Open Access. DOI: 10.1007/s12665-024-11832-7. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85202876737&doi=10.1007%2fs12665-024-11832-7&partnerID=40&md5=ae5b196c808b7cbb8fa1cee7d93d3ad8.

[4] F. Claret et al. "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". In: Frontiers in Nuclear Engineering 3 (2024). Cited by: 7; All Open Access, Gold Open Access. DOI: 10.3389/fnuen.2024.1437714. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85214023365&doi=10.3389%2ffnuen.2024.1437714&partnerID=40&md5=428a4b7fb55008122a93bd29437c6235.

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