

EURAD GAS#HITEC: PhD School

From Workflows towards Digital Twins: OpenWorkFlow-Project

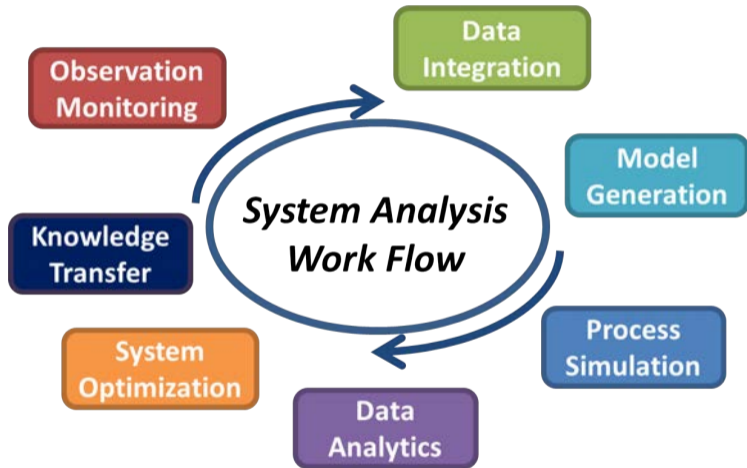
Olaf Kolditz, Norbert Grunwald, Christoph Lehmann & OpenGeoSys
Team

29.08.2023, Liège, Belgium

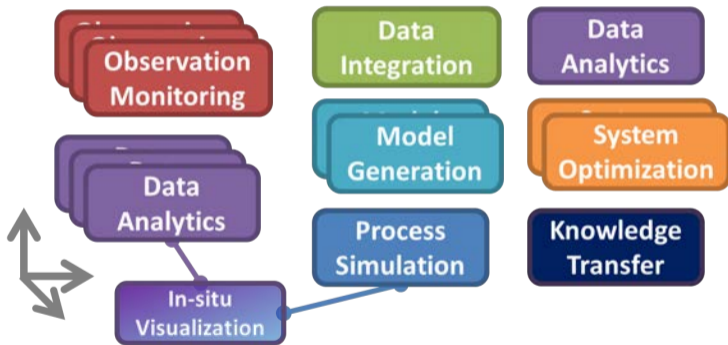
Workflows

Generic Workflows

“A workflow consists of an orchestrated and **repeatable pattern of activity**, enabled by the systematic organization of resources into processes that transform materials, provide services, or **process information.**”
(Wikipedia)



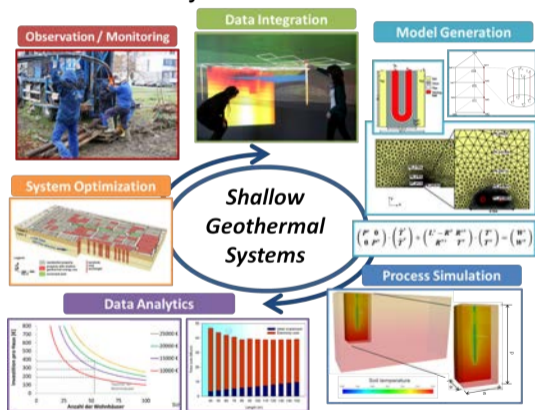
Generic Workflows



- Exchangeable modules >> Pipelines
- Platform-independent
- Script-based environments (Jupyter, web-browser applications)

Specific Workflows

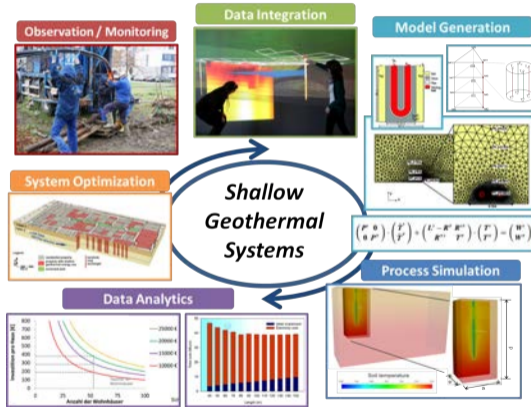
Geothermal Systems



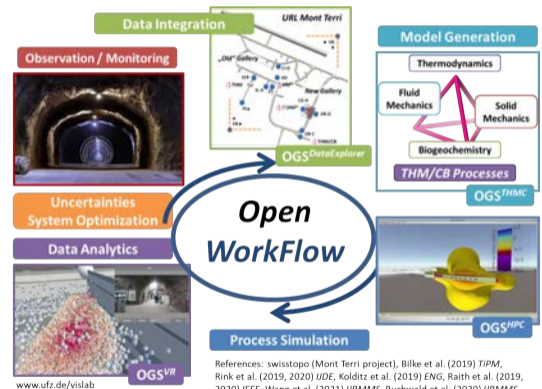
Geotechnical Systems

Specific Workflows

Geothermal Systems



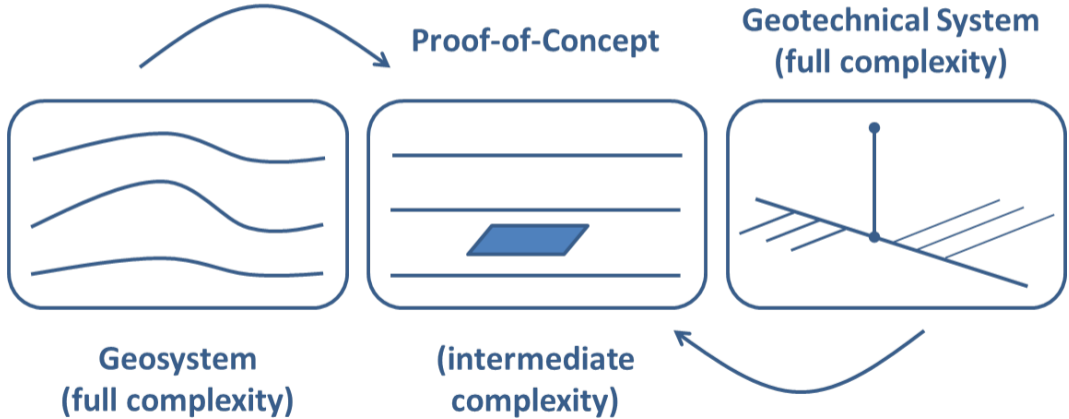
Geotechnical Systems



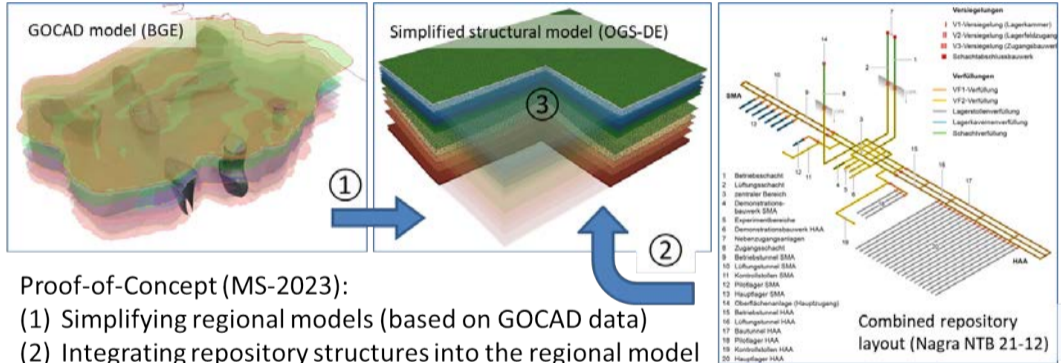
References: swisstopo (Mont Terri project), Bilke et al. (2019) TIPM, Rink et al. (2019, 2020) IJDE, Kolditz et al. (2019) ENG, Raith et al. (2019, 2020) IEEE, Wang et al. (2021) IJRMMS, Buchwald et al. (2020) IJRMMS

- existing interfaces (OGS DataExplorer), level of automation is low ...

Generic Workflow for the Siting Process #1



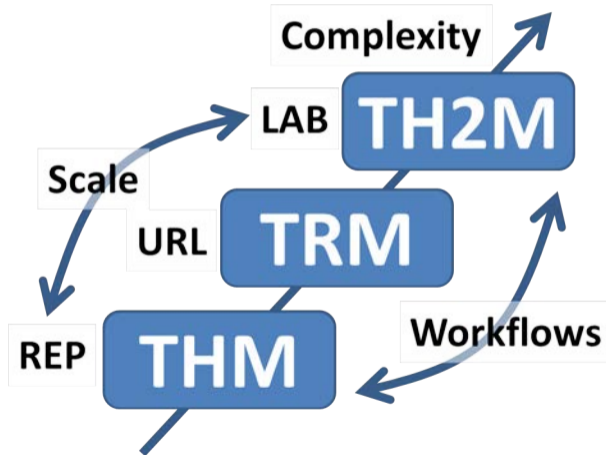
Specific Workflow for the Siting Process #2



Proof-of-Concept (MS-2023):

- (1) Simplifying regional models (based on GOCAD data)
- (2) Integrating repository structures into the regional model
- (3) THMC simulations at various scales and complexity levels (near/far field processes)

Process Selection: Complexity and Scales



OpenGeoSys (OGS)

OpenGeoSys - THMC/RTP Simulator (www.opengeosys.org)

OpenGeoSys

Releases Docs Publications Discourse

Search this site

OpenGeoSys

OPEN-SOURCE MULTI-PHYSICS

OpenGeoSys (OGS) is a scientific [open source project](#) for the development of numerical methods for the simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media. Current version is OpenGeoSys-6 which is documented on this page. For information about OpenGeoSys-5, see [its dedicated section](#). OGS has been successfully applied in the fields of regional, contaminant and coastal hydrology, fundamental and geothermal energy systems, geotechnical engineering, energy storage, CO2 sequestration/storage and nuclear waste management and disposal.

Announcements & Discussions

[OGS Community Meeting 2023 - Safe the data: 21-22.11.2023 in Leipzig](#)



by Lars Bilke
July 28, 2023

[OpenGeoSys 6.4.4 released!](#)



by Lars Bilke
March 10, 2023

[First ogstools release!](#)



by Lars Bilke
January 13, 2023

[1D Heat Conduction problem](#)



by Sherlock
August 24, 2023 · 5 comments

[AttributeError: module 'ogs' has no attribute 'BoundaryCondition'](#)



by Sabrina
August 16, 2023 · 1 comment

[Error: ModuleNotFoundError: No module named 'OpenGeoSys'](#)



by R.Y
August 15, 2023 · 1 comment

Features

OpenGeoSys' adaptable and modular architecture enables a wide variety of use cases and flexible workflows. In the following we highlight some of its most important features.

Books & Tutorials (OGS5)



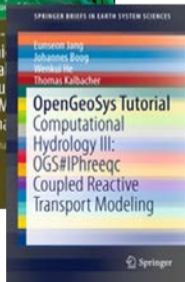
OpenGeoSys



Springer



Springer



Springer

DECOVALEX
2015
DECOVALEX
2019

OpenGeoSys - THMC/RTP Simulator (www.opengeosys.org)

The screenshot shows the OpenGeoSys website homepage. At the top, there are navigation links for 'Releases', 'Docs', 'Publications', and 'Discourse', along with a search bar. The main heading is 'OpenGeoSys' with the tagline 'OPEN-SOURCE MULTI-PHYSICS'. Below this, a paragraph describes the simulator as a scientific open-source project for developing numerical methods for thermo-hydro-mechanical-chemical (THMC) processes. It mentions the current version is OpenGeoSys-6 and lists various application fields like regional hydrology, geothermal energy, and CO2 sequestration.

Announcements & Discussions

OGS Community Meeting 2023 – Safe the data: 21-22.11.2023 in Leipzig



by Lars Bilke
July 26, 2023

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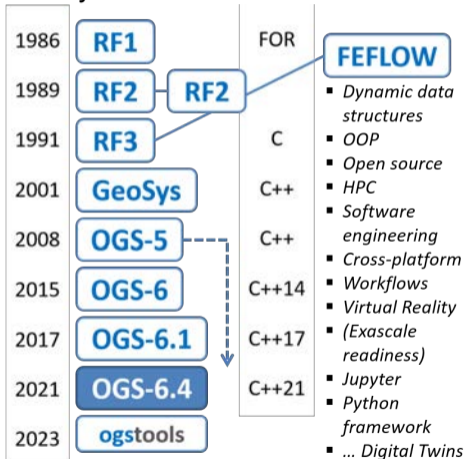


by RY
August 15, 2023 · 1 comment

Features

OpenGeoSys' adaptable and modular architecture enables a wide variety of use cases and flexible workflows. In the following we highlight some of its most important features.

History



OpenGeoSys - Benchmarking Gallery (JupyterLab)

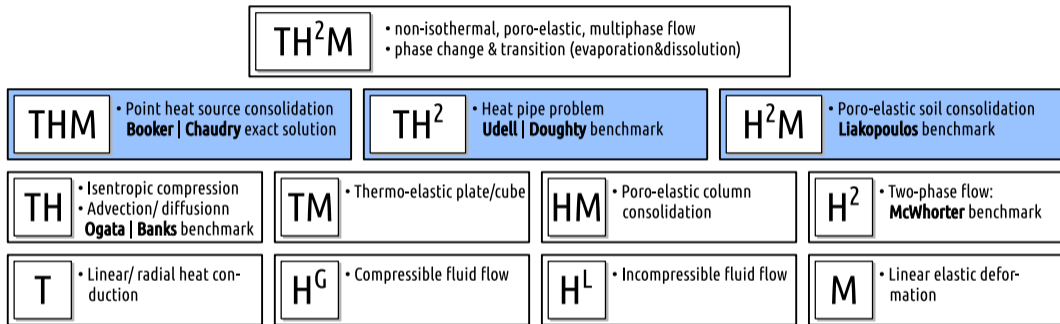
The screenshot displays the OpenGeoSys Benchmarking Gallery interface. On the left, there is a navigation sidebar with categories such as HEAT TRANSPORT BHE, HEAT CONDUCTION, HYDRO MECHANICS, HYDRO-THERMAL, LIQUID FLOW, PHASE FIELD, PYTHON BOUNDARY CONDITIONS, REACTIVE TRANSPORT, RICHARDS FLOW, RICHARDS MECHANICS, SMALL DEFORMATIONS, STEADY STATE DIFFUSION, STORES FLOW, TH2M, THERMAL TWO-PHASE FLOW, THERMO-HYDRO-MECHANICS, THERMO-MECHANICAL PHASE FIELD, THERMO-MECHANICS, THERMO-RICHARDS MECHANICS, and TWO-PHASE FLOW. The main content area is divided into two sections: 'Featured Processes' and 'All Processes'. Each process is represented by a thumbnail image showing a cross-section or a 3D visualization of a geological model, with a small icon and a label below it. The 'Featured Processes' section includes Heat Transport BHE, Reactive Transport, and TH2M. The 'All Processes' section includes Heat Transport BHE, Heat Conduction, Hydro Mechanics, Hydro Component, Hydro Thermal, Liquid Flow, Phase Field, Python Boundary Conditions, Reactive Transport, Richards Flow, Richards Mechanics, Small Deformations, Steady State Diffusion, Stokes Flow, TH2M, and Thermal Two-Phase Flow.

OGS-TH2M Model Class

The screenshot displays the OpenGeoSys Benchmarking Gallery interface for the TH2M model class. The main content area shows the 'TH2M' benchmark hierarchy, which is a collection of 12 sub-benchmarks. Each sub-benchmark is represented by a thumbnail image showing a cross-section or a 3D visualization of a geological model, with a small icon and a label below it. The sub-benchmarks are: Gas Diffusion, Confined Gas Compression, Phase Appearance/Disappearance, McWhorter & Sunada Problem, Ogilby Banks Problem, Heat pipe verification problem, H2M Luikowitsch benchmark, and Pore Pressure Problem. The interface also includes a search bar and a navigation sidebar on the left.

References: [Gru+22], [Pit+23b]

Simulation of Coupled Multiphysics Processes: OpenGeoSys-6 TH2M



References: [Gru+22], [Pit+23b]

OGS participation in DECOVALEX

Lab scale

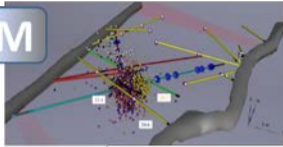
GREAT Cell Experiments



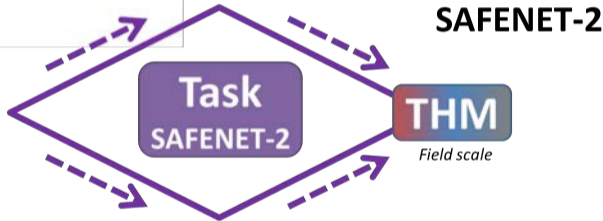
KICT Experiments



HM



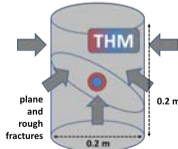
STIMTEC experiment at
URL Reiche Zeche
(Germany)



SAFENET-2

THM

Field scale



Methodology:

- THM fracture mechanics
- Interactive benchmarking (web-based Jupyter notebooks)
- Machine learning for building surrogate models



References:

[Mol+23]

[Rad+23a]

[Rad+23b]

[Pit+23a] (BenVaSim)

Simulation of Coupled Multiphysics Processes (>> Norbert)

A monolithic thermo-hydro-mechanical two-phase flow formulation for modelling gas migration in geotechnical barriers

N. Grunwald^{1,2}, M. Pitz^{3,4}, J. Maßmann³, D. Naumov³, T. Nagel³, O. Kolditz^{5,6}

¹Technische Universität Braunschweig (TU Braunschweig), ²Bundesanstalt für Geowissenschaften und Rohstoffe (BGR), ³Technische Universität Bergakademie Freiberg (TU Bergakademie), ⁴Technische Universität Clausthal (TU Clausthal), ⁵Technische Universität München (TUM), ⁶Technische Universität Dresden (TU Dresden)



Motivation. Various processes in HDR repositories, such as the corrosion of containers, can result in the formation of gaseous hydrogen. This can lead to a buildup of gas pressure in the repository, which could affect the integrity of the artificial and natural barriers. Gas pressure and gas production rate determine the nature of gas transport mechanisms in low-permeability media.

Aim. Gas transport processes in low-permeability clay material were distinguished into four types by Marschall et al. (2005) (see Fig. 1).

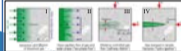


Fig. 1. The main gas transport processes in low-permeability porous media as described by Marschall et al. (2005) (see Fig. 1).

- I. Dissolved gas transport by diffusion and/or advection in the liquid phase.
- II. Formation of separate gas phase, selective transport, and moving gas phase and its dissolved form.
- III. Gas pressure exceeds the tensile strength of the medium, fractures occur and preferential flow paths develop.
- IV. Gas pressure exceeds the tensile strength of the medium, fractures occur and preferential flow paths develop.

Methods. The coupled TH2M formulation of the OpenGeoSys multi-physics solver is used to model transport processes of types II to IV. The latest OpenGeoSys implementation features...

- Compositional two-phase flow (two components)
- Consistent thermodynamics
- Geomechanics
- Massively coupled
- All phases (solid phase, two fluid phases) are compressible
- Phase transitions between the fluid phases (see Fig. 2)

The advantage of coupled processes is that transport and stress states can be calculated simultaneously. Thus, on the one hand, the barrier integrity can be evaluated, and on the other hand, stress or stress-dependent transport properties can be taken into account.

A detailed description of the implementation can be found in [4].

Proof-of-Concept. Single benchmarks will serve as proof-of-concept to demonstrate the usability of the model. In the present case, the transport processes of types I and II are to be examined. The aim of this test is to show the transition from single-phase to two-phase flow regimes.



Fig. 2. Gas saturation over time.

Initial conditions.
 $p_0 = 10^5 \text{ Pa}$
 $p_{\text{sat}} = 10^6 \text{ Pa}$
 $T = 300 \text{ K}$
 $\mu = 0 \text{ m}$

Boundary conditions.
 $\sigma = 31.2 \text{ MPa}$ at $x = 0$
 $\sigma = 0$ at $x = L$
 $\sigma = 0$ at $x = L$
 $\sigma = 0$ at $x = L$
 $\sigma = 0$ at $x = L$

Material properties. OpenGeoSys (OGS) uses the following material properties:
 $\kappa = 10^{-15} \text{ m}^2 \text{ s}^{-1}$
 $\alpha = 0.15$
 $\beta = 1.2 \times 10^{-10} \text{ m}^3 \text{ kg}^{-1}$
 $\gamma = 10^4 \text{ Pa}^{-1}$
 $\mu = 1.2 \times 10^{-10} \text{ m}^3 \text{ kg}^{-1}$
 $\nu = 0.15$
 $\rho = 10^3 \text{ kg m}^{-3}$

Results. In the following diagram, saturation, pressure, and mass fluxes at the left boundary of the domain are plotted over time. The gas transport mechanisms (I, II, III, IV) change from type I to type II in the process.

For about 20 years, all hydrogen is dissolved in the liquid phase and transport conditions prevail. After that time, the increasing viscosity of the water is reached and a gas phase appears.



Fig. 3. Gas saturation over time.

Before the appearance of the gas phase, the gas pressure has no physical meaning except for a possible increase above the content of dissolved gas.

The water pressure hardly changes at all during the time, whereas, it rises to another 20 years and reaches its maximum at its initial level.



Fig. 4. Gas and liquid pressure over time.

During the single-phase regime, almost the entire gas transport is achieved by diffusion in the liquid phase. The advective transport is negligible until it reaches its maximum after the appearance of the gas phase as advective pressure gradient develops. The advective mass flux in the gas phase increases with time and reaches its maximum at the end of the time interval.



Fig. 5. Mass flux over time pressure over time.

References.

- [1] Marschall, A. et al., 2005. Characterisation of gas transport properties of the synthetic clay, a potential near rock formation for radioactive waste disposal. *Journal of Nuclear Energy and Technology - Part B*, 40, 121-139.
- [2] Gao, K. et al., 2014. Experimental observations of mechanical dilation at the onset of gas flow in Callovo-Chalons claystone. In: *Proceedings of the 11th International Conference on Environmental and Engineering Geotechnics*, London, Special Publications 493, 501-516.
- [3] Kolditz, O. et al., 2012. Development of open-source porous media simulation: Principles and experiments. *Transport in porous media*, 135(1), 33-61.
- [4] Grunwald, N. et al., 2022. Geo-mechanical two-phase flow in deformable porous media: Systematic open source implementation and verification procedure. *Geotechnical Engineering, Geophysics, Geomechanics*, 8(3), 1-26.

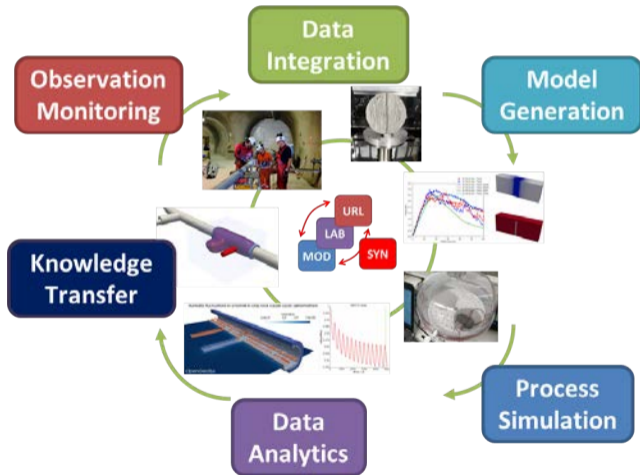
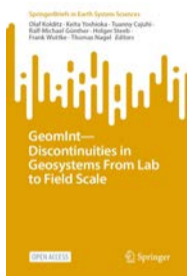
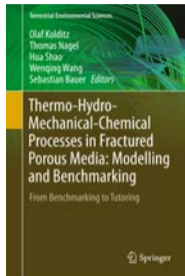
OpenGeoSys-6 TH2M

- Compositional two-phase flow
- Geomechanics (inelastic solids)
- Consistent thermodynamics
- Phase transitions
- Hierarchic benchmarking
- ...

Capable to verify the concept of P. Marschall [MHG05] for various clay types (OPA, COx, Boom)

References: [Gru+22], [Pit+23b]

OpenGeoSys - Applications



OpenGeoSys - Applications

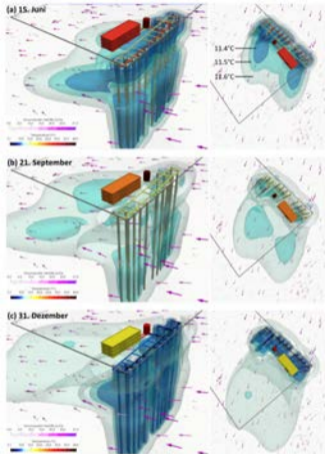
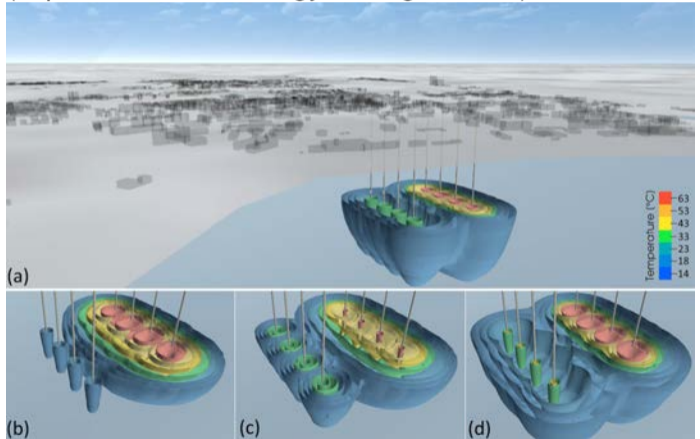


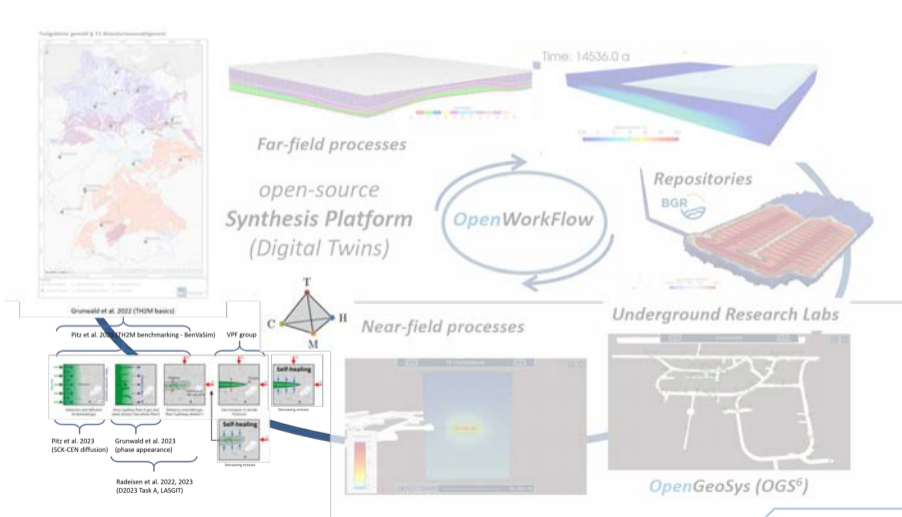
Abbildung 7.6: Visualisierung der Ergebnisse der gekoppelten Simulation von OpenGeoSys und SimulationX. Dargestellt sind die Temperaturentwicklungen in einem Schulgebäude, der zugehörigen Anlage, Wärmesenden und den verbindenden Leitungen via SimulationX sowie von Grundwasserfluss und Temperatur im Untergrund via OpenGeoSys an drei ausgewählten Tagen. Die Transferfunktion der Temperaturdarstellung ist zur besseren Vergleichbarkeit konstant über alle Zeitschritte und dargestellten Komponenten. Die zur Illustration der Temperaturveränderung visualisierten Isotemperaturflächen liegen bei 11.4°C, 11.5°C und 11.6°C (siehe auch Abb. (a) rechts).

Shallow geothermal systems (Leipzig) and ATES (Aquifer Thermal Energy Storage in Kiel)

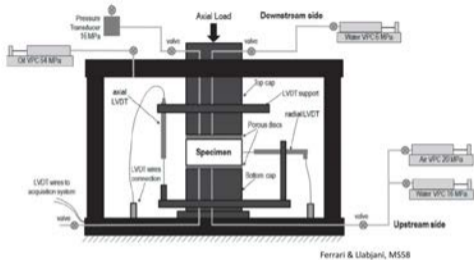


Workflows (cont.)

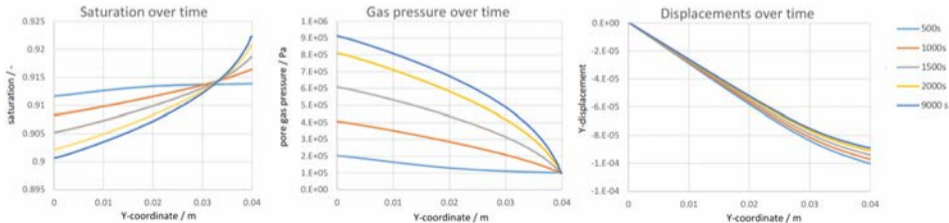
Specific Workflow for the Siting and Repository Concepts #3a



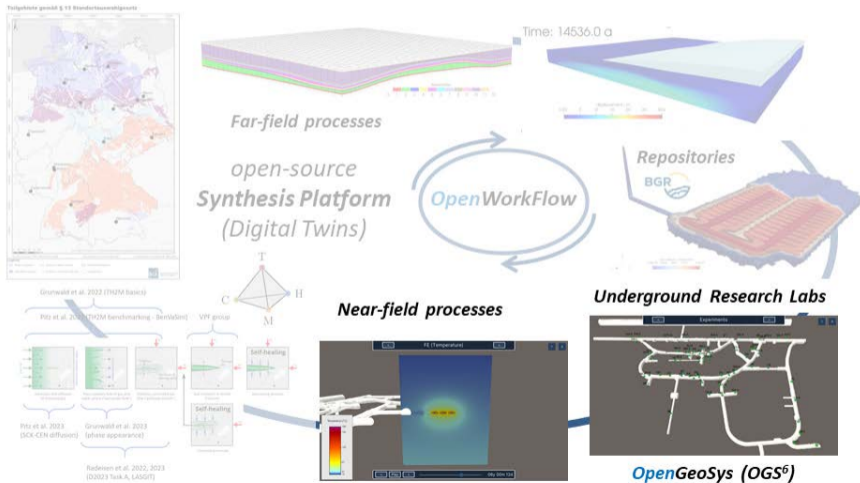
Scale – Lab (EPFL-Experiment, EURAD GAS)



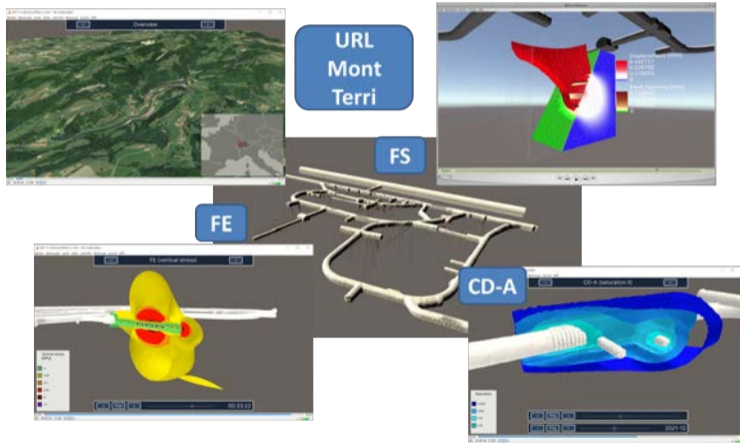
- Aim: Identification of Opalinus Clay properties
- Water Retention behaviour
- Stress-strain relations in relation to gas invasion processes
- Gas transport properties
- Strain dependent permeability model



Specific Workflow for the Siting and Repository Concepts #3b

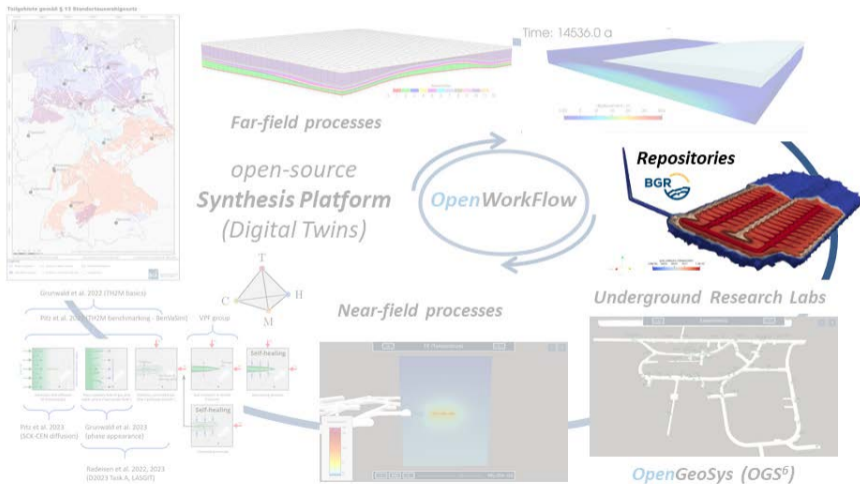


Scale – URL (Mont Terri)



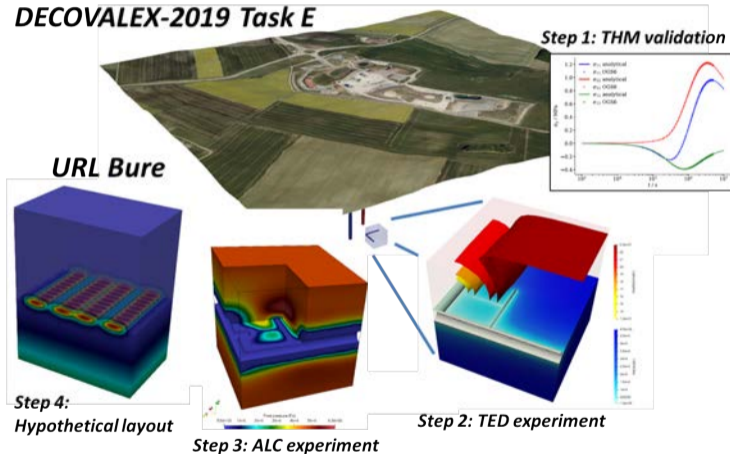
References/Credits: BGR (CD-A, Modeler [Zie+22]), TUBAF (FS, Modeler), UFZ (FE, Wenqing Wang), VIS (Nico Graebing/Karsten Rink) [Gra+22] / GeomInt and iCROSS projects

Specific Workflow for the Siting and Repository Concepts #3c

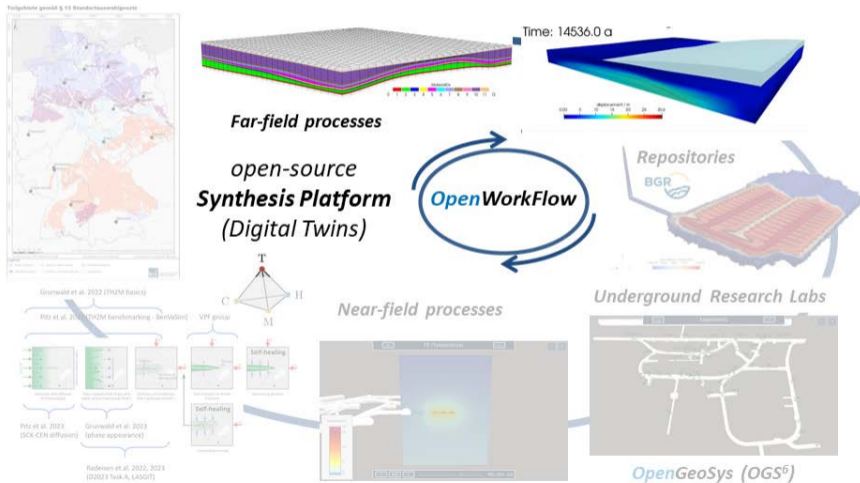


Scale – up to Repository Scale

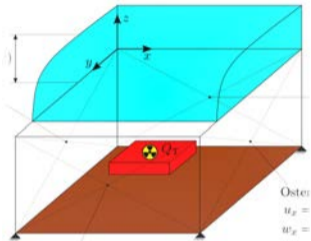
DECOVALEX-2019 Task E



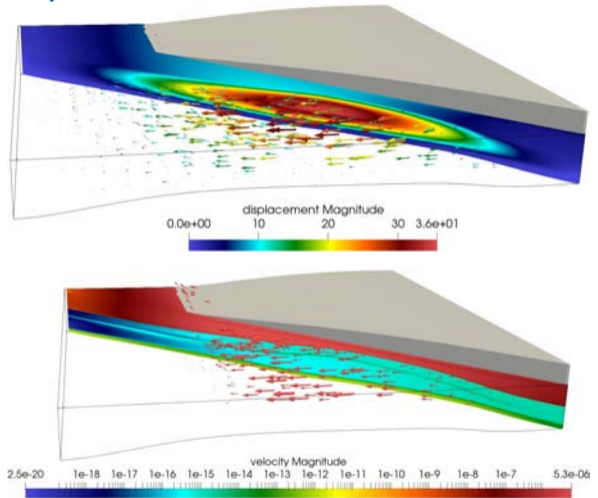
Specific Workflow for the Siting and Repository Concepts #3d



Scale – Far Field Aspects (Glaciation)



- simulation of several glaciation periods
- clay and salt



References/Credits: Florian Zill [Zil+21], AREHS Team

Digital Twins

Digital Twins

“A digital twin is a virtual representation that serves as the **real-time** digital counterpart of a physical object or process.”
(Wikipedia)

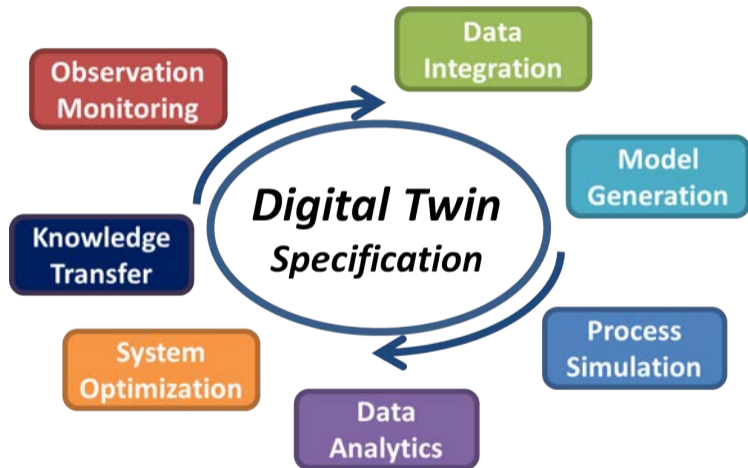


https://commons.wikimedia.org/wiki/File:Oil_rig_Jan_23.jpg

© CC-BY-SA 4.0 SumitAwinash

- describes all relevant properties of that object/process
- shows all relevant behaviours of that object/process
- provides all necessary data via a uniform interface
- ...

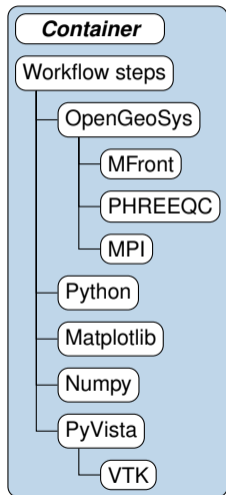
Digital Twin as Workflow Application



Specifications:

- URL Information System (Mont Terri)
- Repository construction (BIM)
- **Model validation (DT2)**
- ...

Software Engineering (DT1)

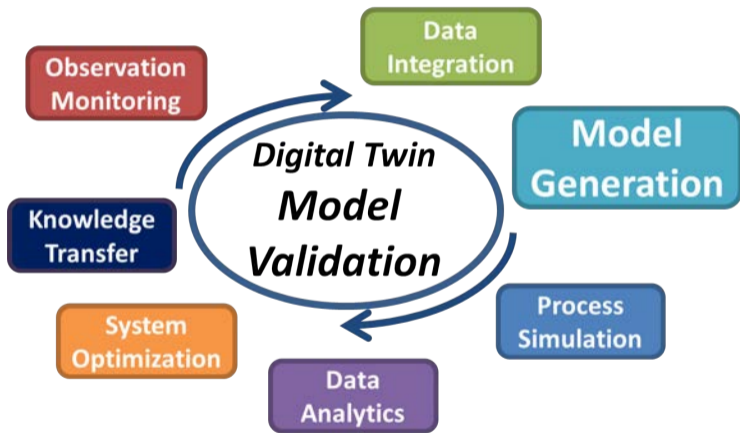


Technical frameworks for DTs

- container = lightweight VM
 - ▶ VM = app + 2nd OS files + 2nd OS processes
 - ▶ container = app + 2nd OS files
- distribute software along with all dependencies
- unified runtime environment
- executable in many different environments
- facilitates reuse of workflow steps
- simplifies adoption by new users

References: [Bil+19]

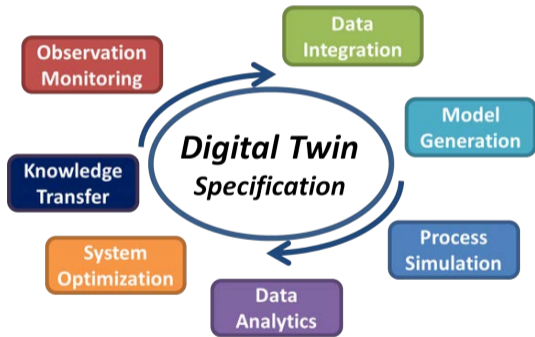
Digital Twin for Model Validation (Upscaling)



Model validation:

- Model generation
- Benchmarking (data integration, code comparison, ...)
- Model scaling
- ...

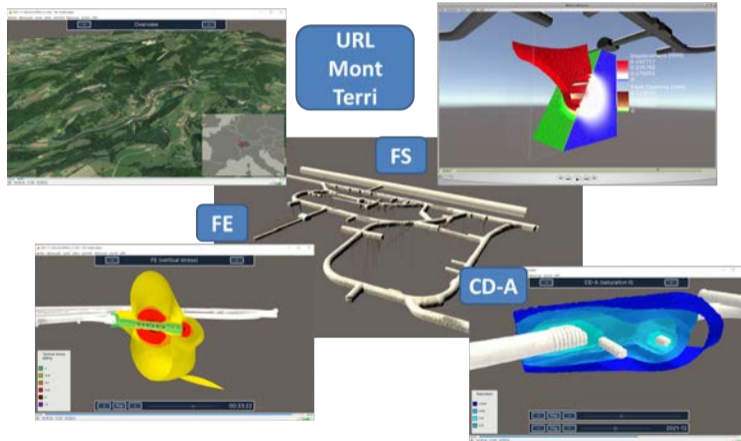
From Workflow Application Towards Digital Twins



WF Flexibility >> DT Specification

- on-the-fly model parameter update
- monitoring of the repository
- continuous model validation
- distributed: multi-agent implementation
- versions
- composability: build more complex twins from a common core
- workflow integration
- need for a robust basis
- ...

Digital Twin VR Application – URL (Mont Terri)



see VISLAB applications and OGS YouTube Channel

Contributors

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Wenqing Wang
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Bundesamt für die Sicherheit der nuklearen Entsorgung
Bundesanstalt für Geowissenschaften und Rohstoffe – BGR

References I

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Thank you for your attention.