HELMHOLTZ
Zentrum für Umweltforschung

EURAD GAS#HITEC: PhD School

From Workflows towards Digital Twins: OpenWorkFlow-Project

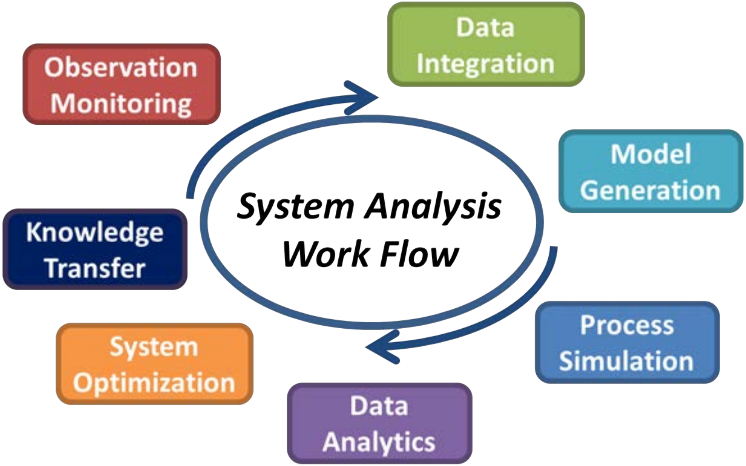
Olaf Kolditz, Norbert Grunwald, Christoph Lehmann & OpenGeoSys Team

29.08.2023, Liège, Belgium

Workflows

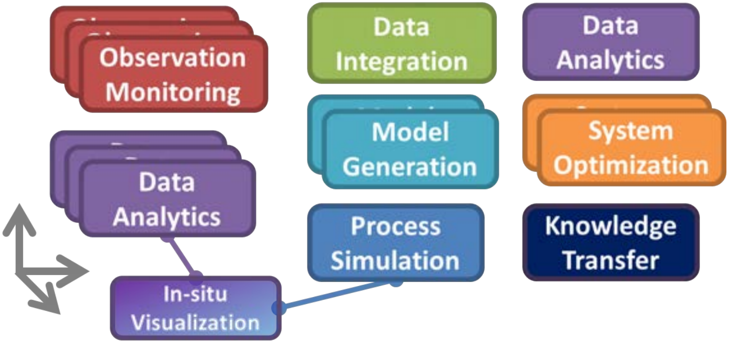
Generic Workflows

"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)



Reference: Ch. Lehmann [LT22], [Kol+19]

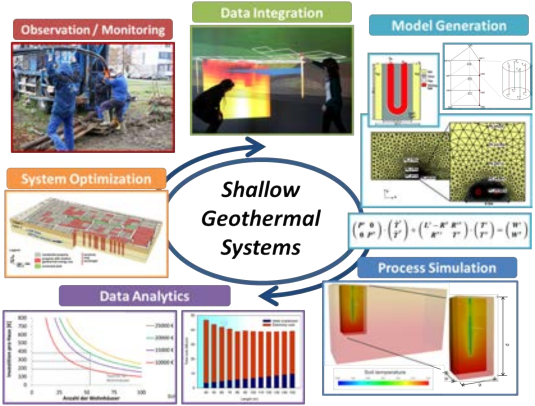
Generic Workflows



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

Specific Workflows

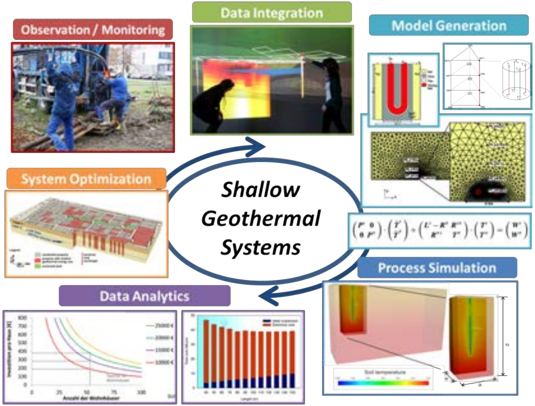
Geothermal Systems



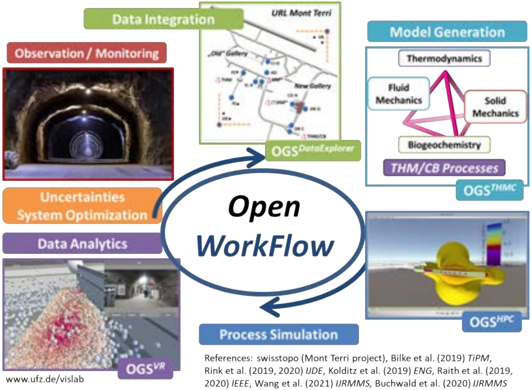
Geotechnical Systems

Specific Workflows

Geothermal Systems



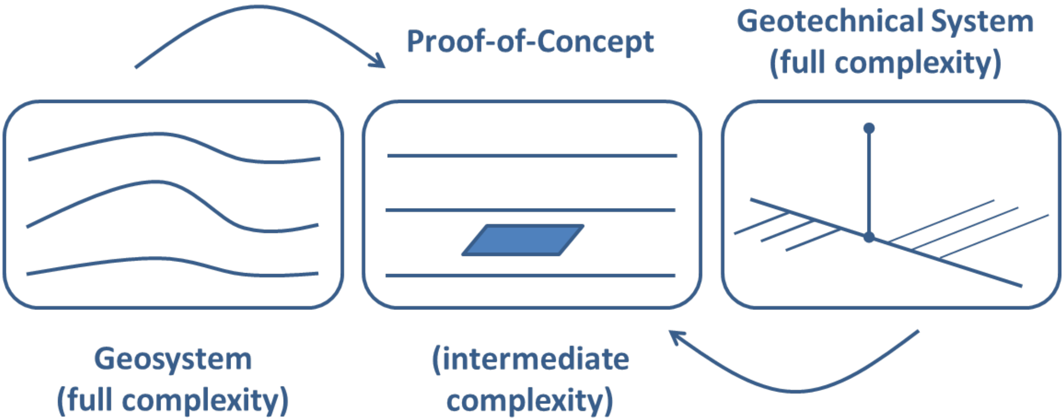
Geotechnical Systems



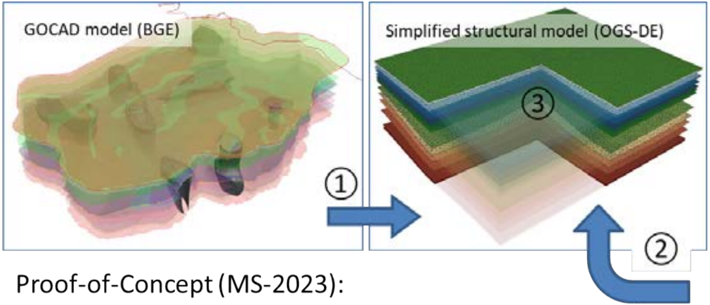
References: swisstopo (Mont Terri project), Bilke et al. (2019) *TiPM*, Rink et al. (2019, 2020) *IJDE*, Kolditz et al. (2019) *ENG*, Raith et al. (2019, 2020) *IEEE*, Wang et al. (2021) *IJRMMS*, Buchwald et al. (2020) *IJRMMS*

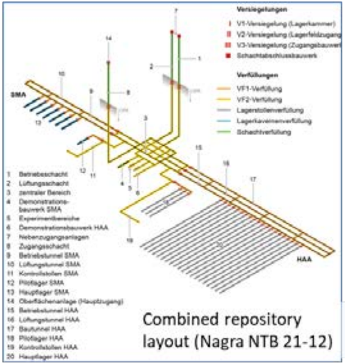
- existing interfaces (OGS DataExplorer), level of automation is low ...

Generic Workflow for the Siting Process #1



Specific Workflow for the Siting Process #2

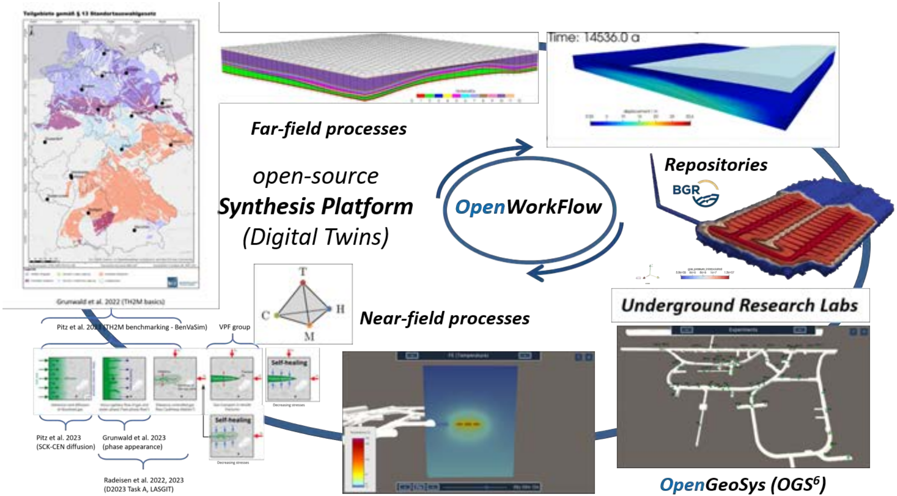




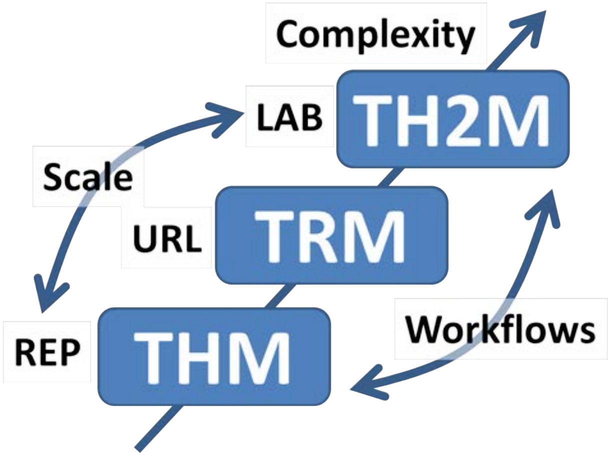
Proof-of-Concept (MS-2023):

(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)

Specific Workflow for the Siting and Repository Concepts #3

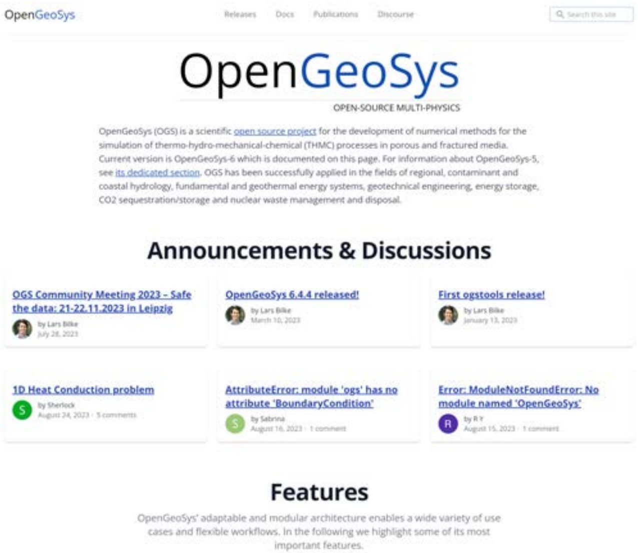


Process Selection: Complexity and Scales



OpenGeoSys (OGS)

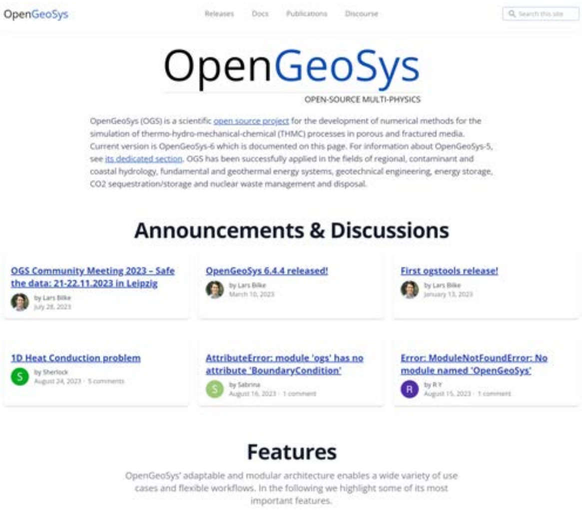
OpenGeoSys - THMC/RTP Simulator (`www.opengeosys.org`)



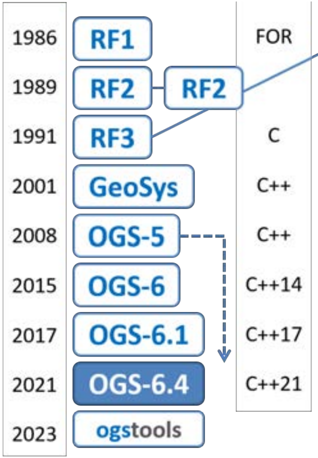
Books & Tutorials (OGS5)

OpenGeoSys

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



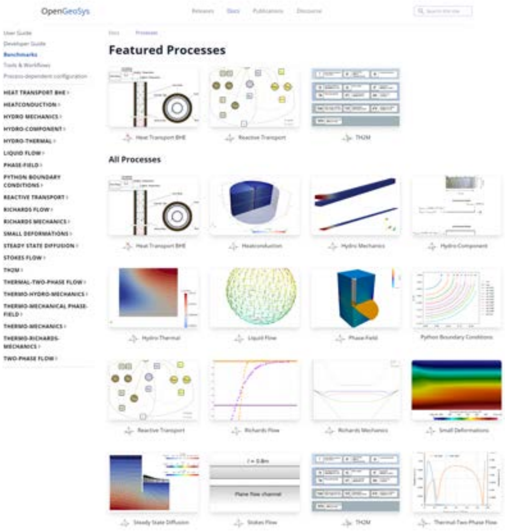
History



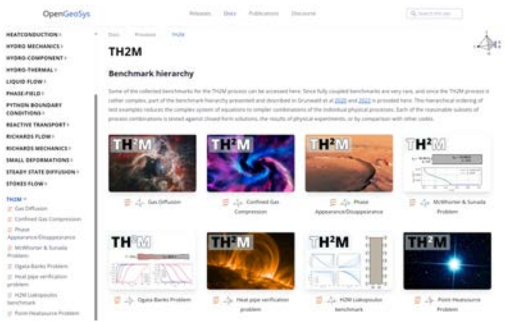
FEFLOW

- *Dynamic data structures*
- *OOP*
- *Open source*
- *HPC*
- *Software engineering*
- *Cross-platform*
- *Workflows*
- *Virtual Reality*
- *(Exascale readiness)*
- *Jupyter*
- *Python framework*
- *... Digital Twins*

OpenGeoSys - Benchmarking Gallery (JupyterLab)



OGS-TH2M Model Class



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

Simulation of Coupled Multiphysics Processes: OpenGeoSys-6 TH2M

TH^2M	• non-isothermal, poro-elastic, multiphase flow • phase change & transition (evaporation&dissolution)

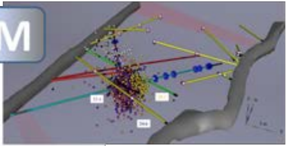
THM	• Point heat source consolidation **Booker | Chaudry** exact solution
TH^2	• Heat pipe problem **Udell | Doughty** benchmark
H^2M	• Poro-elastic soil consolidation **Liakopoulos** benchmark
TH	• Isentropic compression • Advection/ diffusionn **Ogata | Banks** benchmark
TM	• Thermo-elastic plate/cube
HM	• Poro-elastic column consolidation
H^2	• Two-phase flow: **McWhorter** benchmark
T	• Linear/ radial heat conduction
H^G	• Compressible fluid flow
H^L	• Incompressible fluid flow
M	• Linear elastic deformation

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

OGS participation in DECOVALEX

Lab scale
GREAT Cell Experiments

HM



STIMTEC experiment at URL Reiche Zeche (Germany)

SAFENET-2

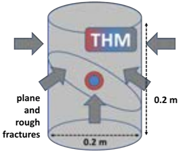
KICT Experiments

THM

Field scale

THM

DECOVALEX 2023



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

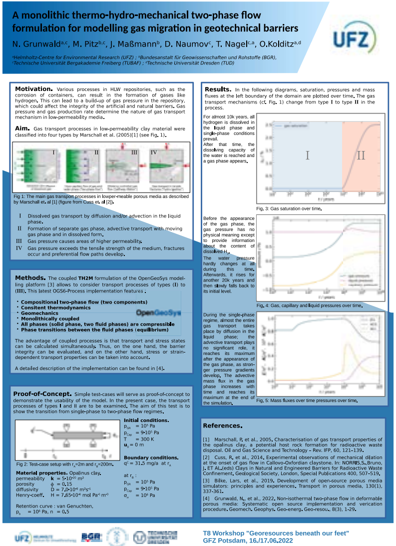
UFZ

STIMTEC

References:
[Mol+23]
[Rad+23a]
[Rad+23b]
[Pit+23a] (BenVaSim)

4

Simulation of Coupled Multiphysics Processes (>> Norbert)



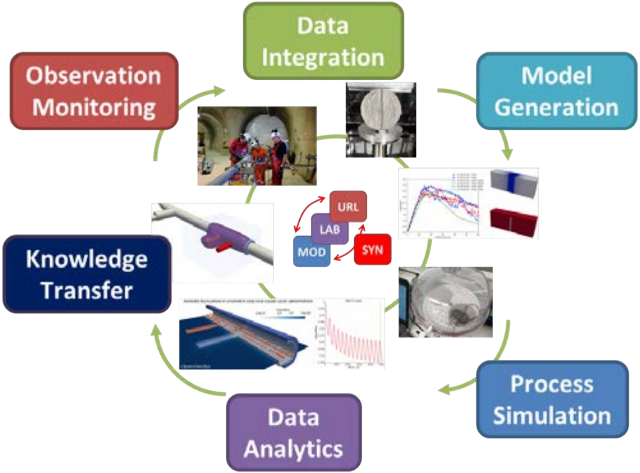
OpenGeoSys-6 TH2M

- 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

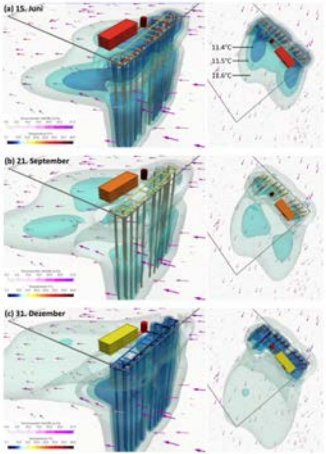
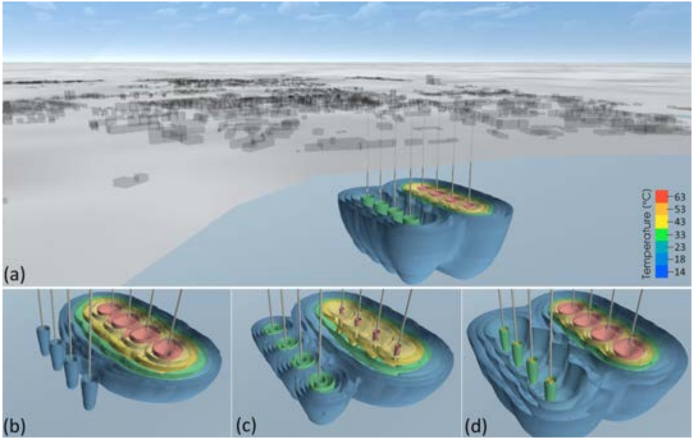


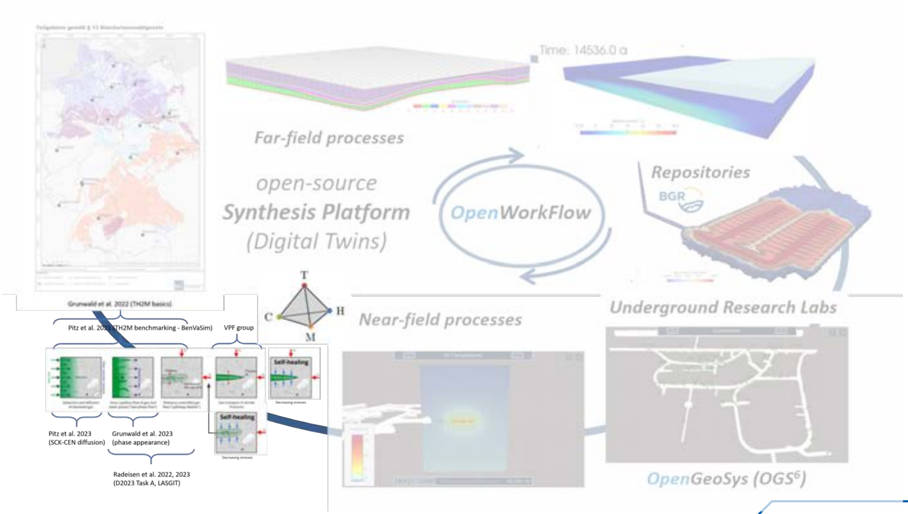
Abbildung 7.6: Visualisierung der Ergebnisse der gekoppelten Simulation von OpenGeoSys und SimulationX. Dargestellt sind die Temperaturentwicklungen in einem Schulgebäude, der zugehörigen Anlage, Wärmesonden und den verbindenden Leitungen via SimulationX sowie von Grundwasserfluss und Temperatur im Untergrund 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)

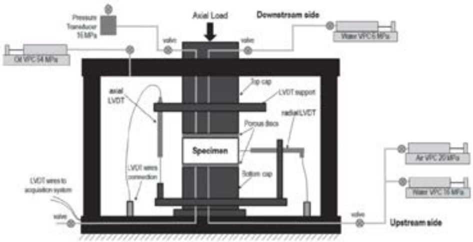


Workflows (cont.)

Specific Workflow for the Siting and Repository Concepts #3a

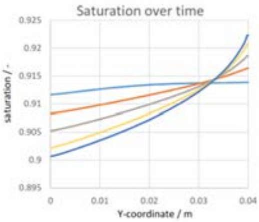


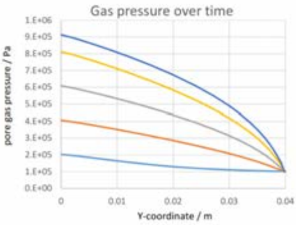
Scale – Lab (EPFL-Experiment, EURAD GAS)

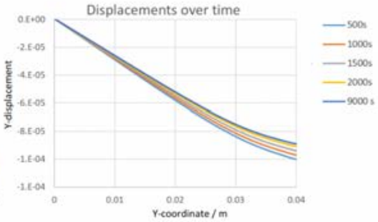


Ferrari & Llabjani, MS58

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

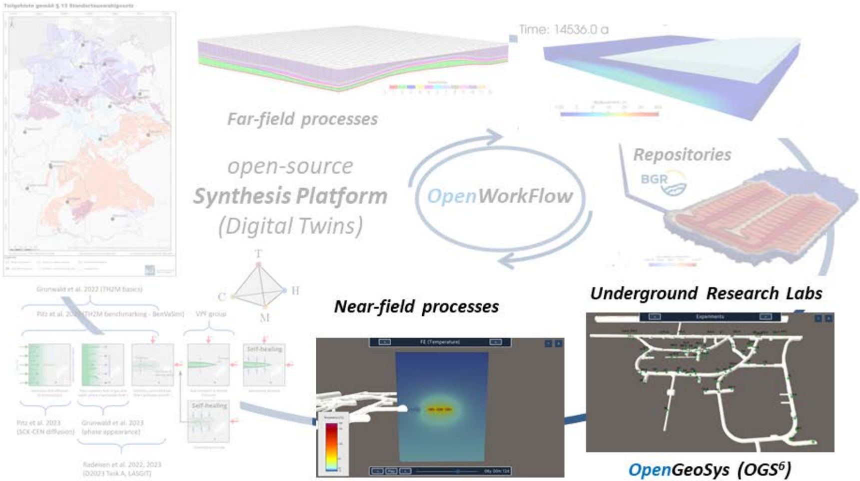




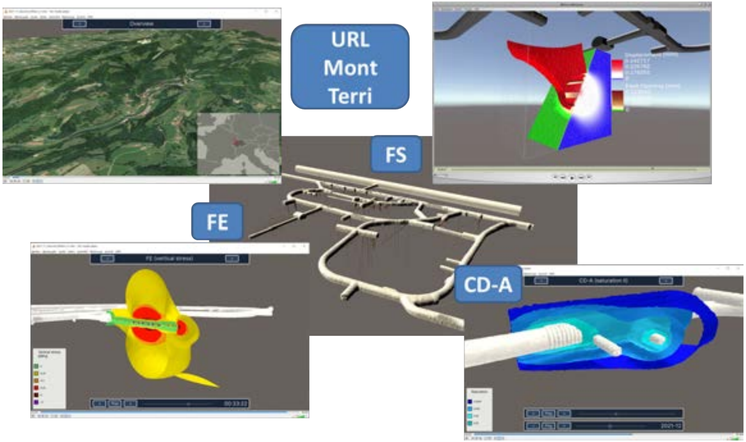


References/Credits: BGR (Michael Pitz [Pit+23b]), EPFL (Alessio Ferrari, Qazim Llabjani)

Specific Workflow for the Siting and Repository Concepts #3b

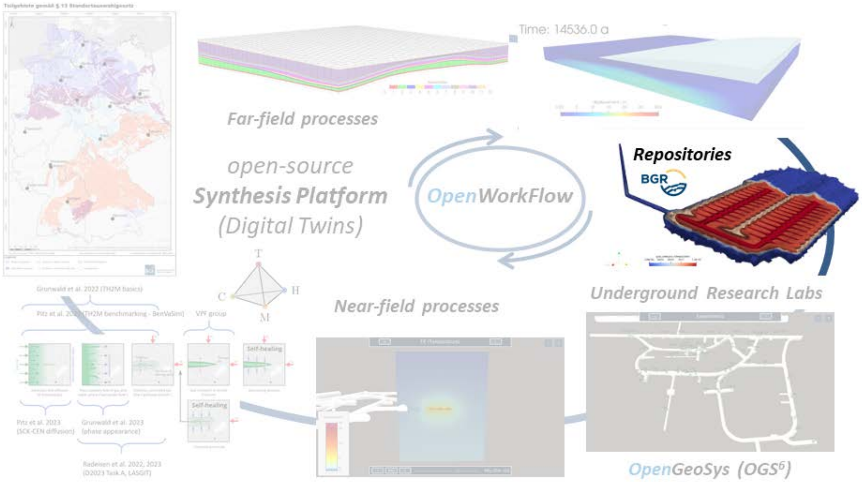


Scale – URL (Mont Terri)

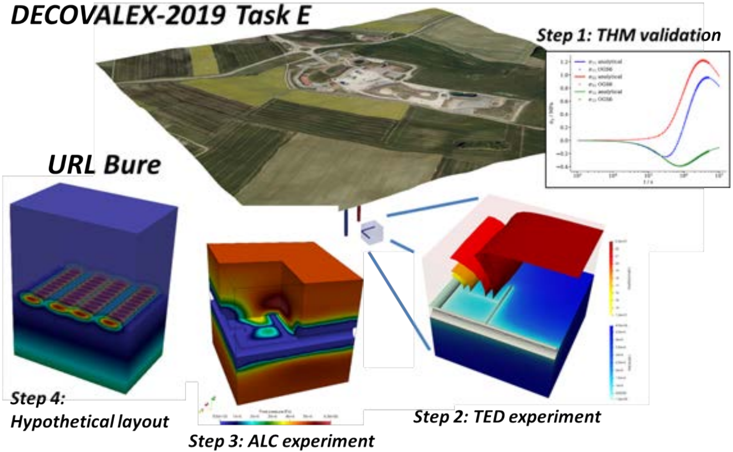


References/Credits: BGR (CD-A, Modeler [Zie+22]), TUBAF (FS, Modeler), UFZ (FE, Wenqing Wang), VIS (Nico Graebling/Karsten Rink) [Gra+22] / GeomInt and iCROSS projects

Specific Workflow for the Siting and Repository Concepts #3c

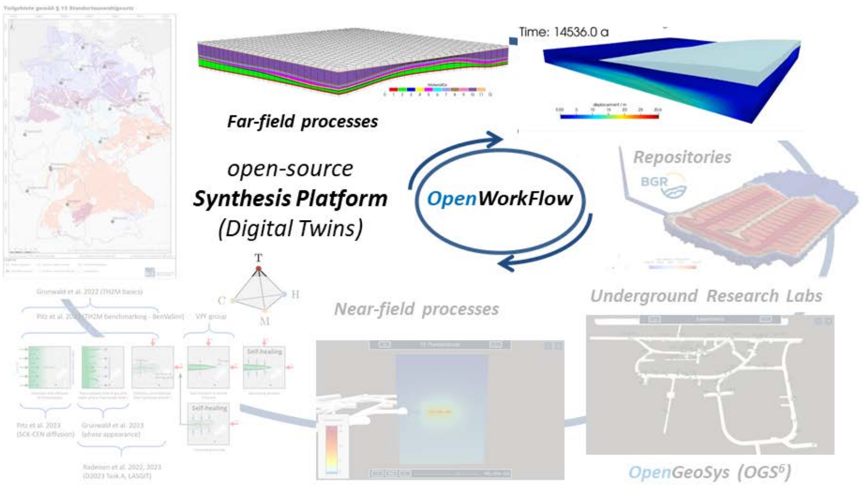


Scale – up to Repository Scale

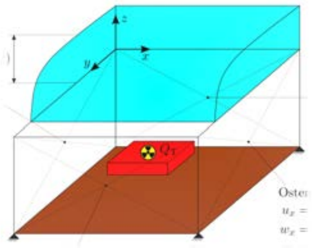


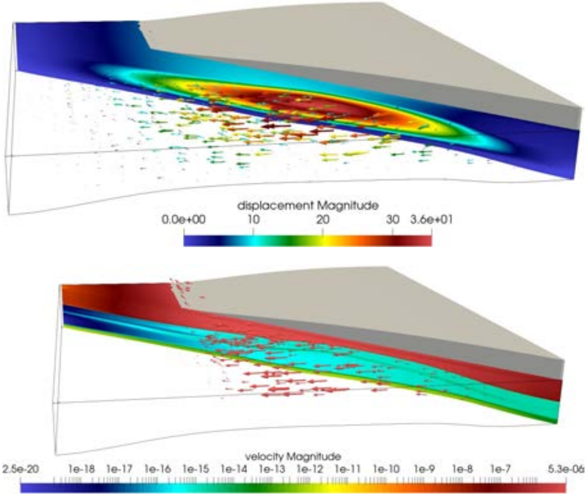
References/Credits: [Wan+21b], [Wan+21a], [Cha+19] / DECOVALEX 2019 project

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

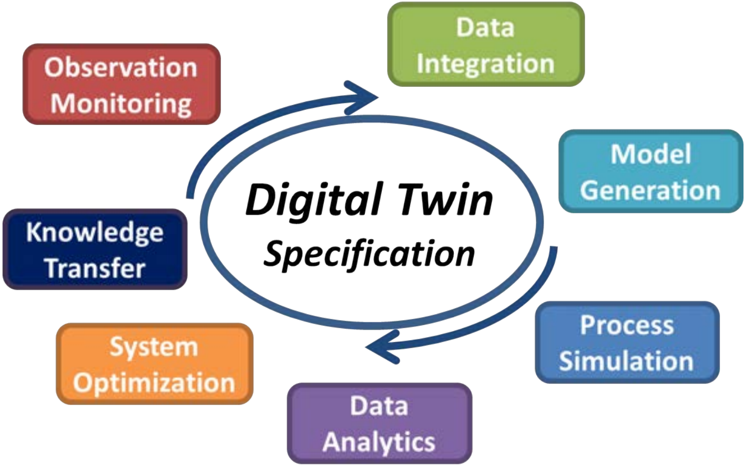
Digital Twins

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

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

- 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



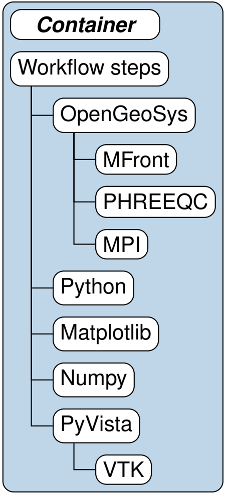
Specifications:

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

Software Engineering (DT1)

References: [Kol+19]

Software Distribution – Container Technology

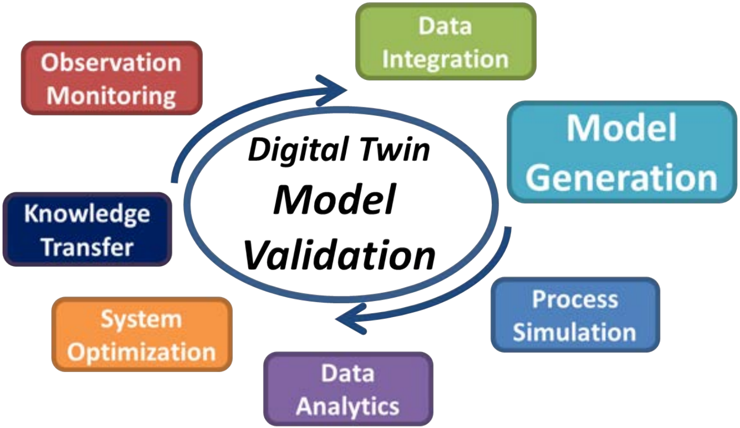


Technical frameworks for DTs

- 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]

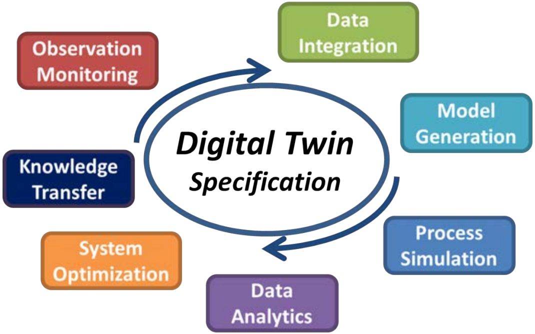
Digital Twin for Model Validation (Upscaling)



Model validation:

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

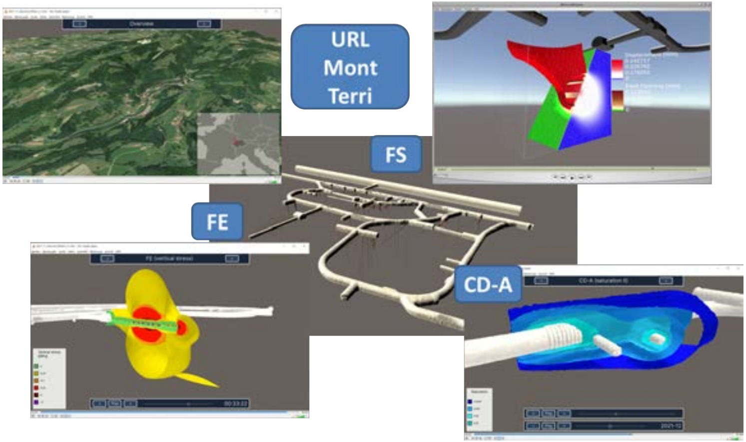
From Workflow Application Towards Digital Twins



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

Lars Bilke
Jörg Buchwald
Aqeel Chaudry
Thomas Fischer
Nico Graebling
Norbert Grunwald
Christoph Lehmann
Renchao Lu
Fabien Magri
Victor Malkovsky
Jobst Maßmann
Tobias Meisel
Thomas Nagel
Dmitri Naumov
Karsten Rink
Ozan Şen
Haibing Shao
Christian Silbermann
Wenqing Wang
Keita Yoshioka
Gesa Ziefle
Florian Zill

Institutions and Acknowledgements

Helmholtz-Zentrum für Umweltforschung – UFZ
TU Bergakademie Freiberg
Bundesgesellschaft für Endlagerung – BGE
Bundesamt für die Sicherheit der nuklearen Entsorgung
Bundesanstalt für Geowissenschafte und Rohstoffe – BGR

References I

[Bil+19] Lars Bilke, Bernd Flemisch, Thomas Kalbacher, Olaf Kolditz, Rainer Helmig, and Thomas Nagel. "Development of Open-Source Porous Media Simulators: Principles and Experiences". In: *Transport in Porous Media* 130.1 (2019). Cited by: 49; All Open Access, Bronze Open Access, pp. 337–361. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85068170902&doi=10.1007%2fs11242-019-01310-1&partnerID=40&md5=33ee985c5c3e4735b93557b9ede5ec1e.

[Cha+19] Aqeel Afzal Chaudhry, Jörg Buchwald, Olaf Kolditz, and Thomas Nagel. "Consolidation around a point heat source (correction and verification)". In: *International Journal for Numerical and Analytical Methods in Geomechanics* 43.18 (2019). Cited by: 10; All Open Access, Hybrid Gold Open Access, pp. 2743–2751. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85073786339&doi=10.1002%2fnag.2998&partnerID=40&md5=4cc9559524aafd722e0ae1082176a8d3.

[Gra+22] Nico Graebling, Ozgür Ozan Şen, Lars Bilke, Tuanny Cajuhi, Dmitri Naumov, Wenqing Wang, Gesa Ziefle, David Jaeggi, Jobst Maßmann, Gerik Scheuermann, Olaf Kolditz, and Karsten Rink. "Prototype of a Virtual Experiment Information System for the Mont Terri Underground Research Laboratory". In: *Frontiers in Earth Science* 10 (2022). Cited by: 1; All Open Access, Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85135239050&doi=10.3389%2ffeart.2022.946627&partnerID=40&md5=98251ecf01b0027598edbacc49fcd4c0.

[Gru+22] Norbert Grunwald, Christoph Lehmann, Jobst Maßmann, Dmitri Naumov, Olaf Kolditz, and Thomas Nagel. "Non-isothermal two-phase flow in deformable porous media: systematic open-source implementation and verification procedure". In: *Geomechanics and Geophysics for Geo-Energy and Geo-Resources* 8.3 (2022). Cited by: 4; All Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85130399620&doi=10.1007%2fs40948-022-00394-2&partnerID=40&md5=6b959574110fc5f4c5df0b773b681be9.

[Kol+19] Olaf Kolditz, Uwe-Jens Gorke, Haibing Shao, Hua Shao, and Thomas Nagel. "Workflows in environmental geotechnics: Status-quo and perspectives". In: *Environmental Science and Engineering* (2019). Cited by: 1, pp. 119–127. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85060653775&doi=10.1007%2f978-981-13-2221-1_6&partnerID=40&md5=9d7f3f14783442ae72089d8e2caef986.

[LT22] Ch. Lehmann and OGS Team. "From Workflows towards Digital Twins". In: *Tage der Standortauswahl* (2022). Keynote talk, Aachen, 08.06.2022.

References II

[MHG05] P. Marschall, S. Horseman, and T. Gimmi. "Characterisation of gas transport properties of the Opalinus Clay, a potential host rock formation for radioactive waste disposal". In: *Oil and Gas Science and Technology* 60.1 (2005), pp. 121–139. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-20544436678&doi=10.2516%2fogst%3a2005008&partnerID=40&md5=a6edfc19bc794ad1325c0da667a66397.

[Mol+23] Mostafa Mollaali, Olaf Kolditz, Mengsu Hu, Chan-Hee Park, Jung-Wook Park, Christopher Ian McDermott, Neil Chittenden, Alexander Bond, Jeoung Seok Yoon, Jian Zhou, Peng-Zhi Pan, Hejuan Liu, Wenbo Hou, Hongwu Lei, Liwei Zhang, Thomas Nagel, Markus Barsch, Wenqing Wang, Son Nguyen, Saeha Kwon, Changsoo Lee, and Keita Yoshioka. "Comparative verification of hydro-mechanical fracture behavior: Task G of international research project DECOVALEX–2023". In: *International Journal of Rock Mechanics and Mining Sciences* 170 (2023). Cited by: 0. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85166325287&doi=10.1016%2fj.ijrmms.2023.105530&partnerID=40&md5=3a43688518353d27ce8a084a093cb90c.

[Pit+23a] Michael Pitz, Norbert Grunwald, Bastian Graupner, Kata Kurgyis, Eike Radeisen, Jobst Maßmann, Gesa Ziefle, Jan Thiedau, and Thomas Nagel. "Benchmarking a new TH2M implementation in OGS-6 with regard to processes relevant for nuclear waste disposal". In: *Environmental Earth Sciences* 82.13 (2023). Cited by: 0; All Open Access, Green Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85163128056&doi=10.1007%2fs12665-023-10971-7&partnerID=40&md5=b7997c7b6d94abe36397c9606861f5fe.

[Pit+23b] Michael Pitz, Sonja Kaiser, Norbert Grunwald, Vinay Kumar, Jörg Buchwald, Wenqing Wang, Dmitri Naumov, Aqeel Afzal Chaudhry, Jobst Maßmann, Jan Thiedau, Olaf Kolditz, and Thomas Nagel. "Non-isothermal consolidation: A systematic evaluation of two implementations based on multiphase and Richards equations". In: *International Journal of Rock Mechanics and Mining Sciences* 170 (2023). Cited by: 0; All Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85167438928&doi=10.1016%2fj.ijrmms.2023.105534&partnerID=40&md5=305d32c2037651ea105488c12ff77d87.

[Rad+23a] Eike Radeisen, Hua Shao, Jürgen Hesser, Olaf Kolditz, Wenjie Xu, and Wenqing Wang. "Simulation of dilatancy-controlled gas migration processes in saturated bentonite using a coupled multiphase flow and elastoplastic H2M model". In: *Journal of Rock Mechanics and Geotechnical Engineering* 15.4 (2023). Cited by: 1; All Open Access, Gold Open Access, pp. 803–813. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85132868396&doi=10.1016%2fj.jrmge.2022.05.011&partnerID=40&md5=d5c9c42b7ddf1da2e7aa9b18fe7e2af6.

References III

[Rad+23b] Eike Radeisen, Hua Shao, Michael Pitz, Jürgen Hesser, and Wenqing Wang. "Derivation of heterogeneous material distributions and their sensitivity to HM-coupled two-phase flow models exemplified with the LASGIT experiment". In: *Environmental Earth Sciences* 82.14 (2023). Cited by: 0; All Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85164116109&doi=10.1007%2fs12665-023-11004-z&partnerID=40&md5=28f99fe6795c19f8302ae83eabd4402c.

[Wan+21a] Wenqing Wang, Hua Shao, Thomas Nagel, and Olaf Kolditz. "Analysis of coupled thermal-hydro-mechanical processes during small scale in situ heater experiment in Callovo-Oxfordian clay rock introducing a failure-index permeability model". In: *International Journal of Rock Mechanics and Mining Sciences* 142 (2021). Cited by: 10; All Open Access, Bronze Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85105047093&doi=10.1016%2fj.ijrmms.2021.104683&partnerID=40&md5=cbcca69cf3806f2de20ecdc4a638ffd6.

[Wan+21b] Wenqing Wang, Hua Shao, Karsten Rink, Thomas Fischer, Olaf Kolditz, and Thomas Nagel. "Analysis of coupled thermal-hydro-mechanical processes in Callovo-Oxfordian clay rock: From full-scale experiments to the repository scale". In: *Engineering Geology* 293 (2021). Cited by: 4; All Open Access, Bronze Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85111874158&doi=10.1016%2fj.enggeo.2021.106265&partnerID=40&md5=a047b4c01c5a9b9c1ace6b8d9a96bc5c.

[Zie+22] G. Ziefle, T. Cajuhi, N. Graebling, D. Jaeggi, O. Kolditz, H. Kunz, J. Maßmann, and K. Rink. "Multi-disciplinary investigation of the hydraulic-mechanically driven convergence behaviour: CD-A twin niches in the Mont Terri Rock Laboratory during the first year". In: *Geomechanics for Energy and the Environment* 31 (2022). Cited by: 5; All Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85126814414&doi=10.1016%2fj.gete.2022.100325&partnerID=40&md5=93000ebc336d62099caa1a7fc9d373a5.

[Zil+21] Florian Zill, Christoph Lüdeling, Olaf Kolditz, and Thomas Nagel. "Hydro-mechanical continuum modelling of fluid percolation through rock salt". In: *International Journal of Rock Mechanics and Mining Sciences* 147 (2021). Cited by: 2; All Open Access, Hybrid Gold Open Access. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-85114935462&doi=10.1016%2fj.ijrmms.2021.104879&partnerID=40&md5=25ca33bca708cddce37005049ae37995.

Thank you for your attention.