

Workflows in  
**Mechanistic Geosystems Analysis**

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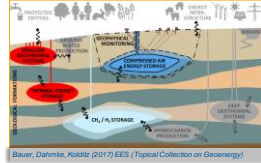
HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH - UFZ

Relevance | Motivation  
**„Energy and Heat Transition“**



- **Solid Earth:** Origin of minerals, fossil fuels, water, rocks and soil
- **Geosystems:** Sufficient and safe space for energy storage and waste repositories
- **Competition|Synergies** in usage concepts

- Challenges**
- Large **storage** capacities for surplus energies from fluctuating renewables (Power to X technologies, 100+ TWh/a.)
  - Safe **repositories** to deposit energy waste, “**Heat Transition**” (50% primary demand): Geothermal systems for urban supply
  - **Need:** Scientific methodology and knowledge-based tools for assessment of subsurface usage concepts: feasibility, decision making, legislation, environmental impacts

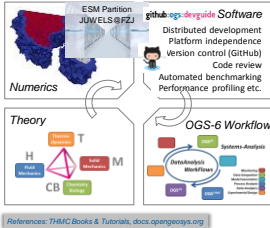


- Approach**
- Developing and providing a **unified mechanistic framework** for a comparative evaluation of different geotechnological options

Framework  
**OpenGeoSys Workflows**



**Our Credo:** *Combining Geosciences and Information Technology for a new generation of scientific codes*



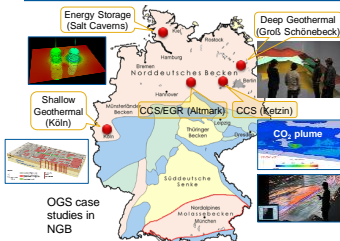
- Theory**
- First Principles, Theory of Porous Media
  - Coupled fluid # solid mechanics and reactive transport processes (THM/CB > PDEs)
- Numerics**
- FEM: Tailored for fractured-porous media and coupled problems
- Software**
- Professional software engineering (> Poster)
  - Designed for new HPC technologies (hybrid)
- OGS-Workflows**
- Data integration # numerical engine # visual data analytics
  - Open source project with almost 30 years experience (permanent renovation)

Framework  
**OpenGeoSys Workflows**



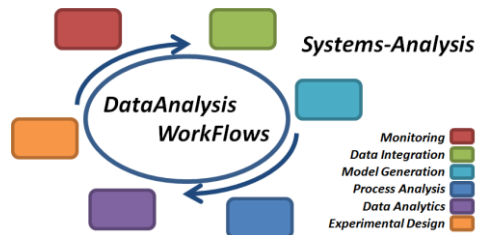
- Use case**
- Rapid project work
  - On demand
- Development**
- OGS DataExplorer
  - OGS Visualization pipelines

Operational Geosystems Modeling  
**Geoenery Applications in Northern Germany**

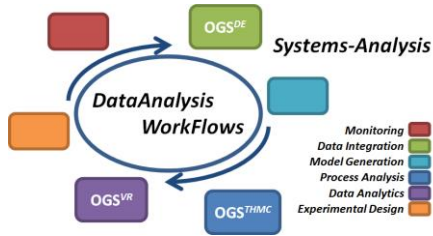


- North-German-Basin (NGB):** Real-scale test bed for Germany's various geoenery applications
- Operational Models**
- CO<sub>2</sub> storage: Ketzin
  - Enhanced Gas Recovery: Altmark
  - Enhanced Geothermal Systems: Groß Schönebeck (Poster session)
  - Energy Storage: Salt caverns
  - Shallow Geothermal (Poster session)
- Transferable Models**

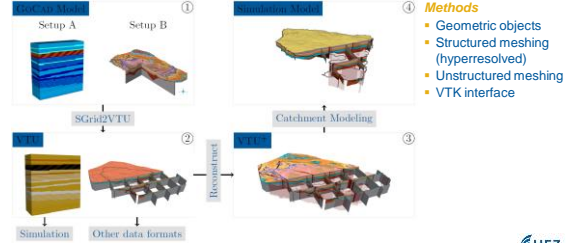
Framework  
**Generic Workflow Concept**



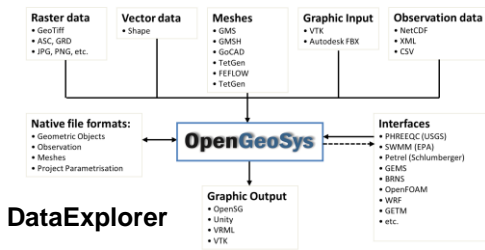
Framework  
Generic Workflow Concept



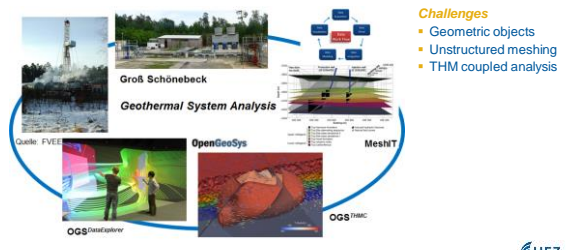
Framework  
Generic Workflow Concept: Topology



Framework  
Generic Workflow Concept: Interfaces



Framework  
Workflow Applications: Geothermal Energy



Example #1  
Enhanced Geothermal Systems (EGS)



**Challenge**

- Fully coupled THM model including all important reservoir elements (sediment layers, faults) and geotechnical features (wellbores, hydro-fracs)

**Achievements and Future Work**

- Reservoir efficiency:** 2nd production wellbore essential for long-term heat extraction
- Reservoir evolution:** Wellbore distance and local stress field orientation are equally important (THM effects)
- Hydrogeochemistry:** Clogging effects are crucial > understanding of THMC processes

**Partners:** GFZ, KIT, UFZ

Watanabe et al. (2018) SpringerBriefs; Jacquoy, Watanabe et al. (2016) Technophysics; Böhnner, Watanabe et al. (2015) Comput. Geosci.

Framework  
Workflow Applications: Geothermal Energy



**Challenges**

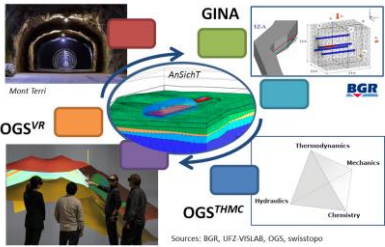
- Conceptual modeling (multi-continua approach)
- Coupling (monolithic)
- Borehole heat exchanger arrays
- Mechanics (THM): Freezing-thawing

**Geothermal System Analysis Workflow**

Efficiency of borehole heat exchanger (BHE)  
Exploit FEM modelling of BHE  
Resolution: >10<sup>6</sup> FE nodes  
Special BHE model development for geothermal well soil/groundwater heat exchange  
Problem size: ~10<sup>7</sup> FE nodes  
After Dierich (2014)



Framework  
Workflow Applications: Geotechnics



- Application areas**
- CO<sub>2</sub> storage
  - Energy storage
  - Waste deposition
- Challenges**
- HPC for field site applications
  - Mechanics: new constitutive models of energy storage – frequent cycling loading / unloading

Sources: BGR, UFZ-VISLAB, OGS, swisstopo



Example #2:  
Carbon Capture Storage (CCS) (T)H<sup>2</sup>M



**Challenges**

- Reservoir models for CO<sub>2</sub> storage sites (Ketzin and Altmark) including multi-phase flow and deformation effects > (T)H<sup>2</sup>M

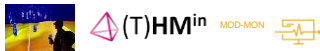
**Achievements**

- Systematic benchmark studies for CO<sub>2</sub> storage (CO<sub>2</sub>BENCH) > extension to 3D
- Physics: Density effects in multiphase flows (sc CO<sub>2</sub> and brines) important for early arrival time calculation
- Computation: HPC methods are essential for field scale applications

References: Park, Böttcher et al. (2012) Comp. Phys.; Kolditz et al. (2012) CO<sub>2</sub>BENCH, EES; McDermott, Wang et al. (2016) Greenhouse Gas Control



Example #3:  
Cavern Energy Storage (T)HM<sup>in</sup>



**Challenges**

- Entire life cycle of cavern
- Realistic cavern geometries
- Typical operation scenarios (frequencies) analyzed

**Achievements and Future Work**

- Newest constitutive salt models for cyclic processes implemented (IfG cooperation)
- Certain operation modes can lead to failure
- Cavern arrays are required for more frequent charging/discharging > interaction

References: Böttcher, Nagel et al. (2017) EES (ANGUS+ Topical Collection); Nagel, Minsky, Böttcher et al. (2017) Comput. Struct.



Example #4:  
Technical Energy Storage T<sup>2</sup>HC<sup>2</sup>



**Challenges**

- High-temperature energy storage (1200°C)
- Extensions for local thermal non-equilibrium processes
- Reactor, material and process to be designed in unison

**Achievements**

- Novel composite material systems numerically investigated (metal-oxides, zeolites)
- Models greatly reduced experimental effort
- OGS - reference model for other groups

References: Lehmann, Nagel et al. (2017) Appl. Energy; Semprini, Nagel et al. (2017) Energy Conv. Manag.; Nagel et al. (2016) Review, Appl. Energy



Framework OGS  
Documentation | Knowledge Transfer



**Benchmarking**

**Tutorials**

**Digital Platforms**

Learn OpenGeoSys

For Users

For Developers

For Everyone

OpenGeoSys

Knowledge & Technology Transfer

Regular Training Courses and Community Meetings

References: THMC Books (vol. 4 dedicated to DECOVALEX) & Tutorials, docs.opengeoSys.org



Subunit: Geosystems Modeling  
Outlook & International Activities



**Nuclear Waste Management:**

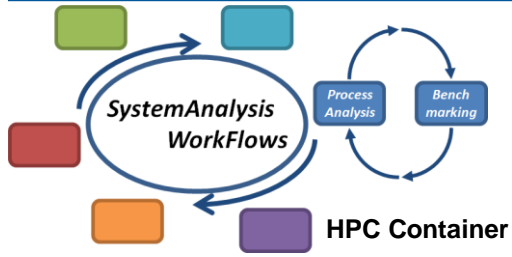
- Feasibility of different host rock types (unified frameworks)
- Concepts for near and far field modeling
- Reactive transport processes (radionuclide migration)

**International Activities**

- Mexico: Superhot geothermal systems
- China: Urban heating/cooling supply

References: Parisio, Nagel et al. (2018) NSR; Lu, Shao et al. (2018) JGR-Solid Earth (submitted)





Thank you for your attention

