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OPENGEOSYS: AN OPEN-SOURCE INITIATIVE FOR NUMERICAL SIMULATION OF THERMO-HYDRO-MECHANICAL/CHEMICAL (THM/C) PROCESSES IN POROUS MEDIA

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In this paper we describe the OpenGeoSys (OGS) project, which is a scientific open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical processes in porous media. The basic concept is to provide a flexible numerical framework (using primarily the Finite Element Method (FEM)) for solving multi-field problems in porous and fractured media for applications in geoscience, hydrology and energy storage. To this purpose OGS is based on an object-oriented FEM concept including a broad spectrum of interfaces for pre- and postprocessing. The OGS idea has been in development since the mid-eighties and has been continuously developed in concept and software implementations evolved through FORTRAN, C, and C++. The idea behind OGS is to provide an open platform to the community, outfitted with professional software-engineering tools such as platform-independent compiling and automated benchmarking. A comprehensive benchmarking book has been published (*Kolditz et al.* [1]), second volume is in print. Benchmarking has been proven to be a valuable tool for cooperation between different developer teams. On one hand, object-orientation (OO) provides a suitable framework for distributed code development; however, the parallelization of OO codes still lacks efficiency. High-performance-computing efficiency of OO codes is subject to future research (*Wang et al.* [2]). Currently, OGS development efforts are dedicated to visual data and model integration for complex hydrological applications (*Rink et al.* [3])

INTRODUCTION

In nature, processes are coupled strongly with each other. Much progress has been achieved towards understanding the complicated processes in deep geological disposal of radioactive waste, CO2 subsurface sequences, geothermal applications and energy storage.

Numerical tools dealing with the coupled thermal, hydraulic, mechanical, chemical and biological processes have been developed to analyze experimental outputs, field observations, laboratory tests. One important issue in the development of numerical codes is of course the code validation and model comparison. Therefore, different international benchmarking projects have been announced for this purpose, such as DECOVALEX project (1992–2015), CO2BENCH, SSBENCH, and Sim-SEQ.

For long-term performance and safety assessment of nuclear waste isolation in deep geological formations, an important issue is the need to guarantee the isolation of an underground repository. To answer this question, radioactive nuclide transport processes under the coupled conditions involving mechanical stability; thermal loading from the high-level waste, and chemistry in the groundwater should be predicted numerically to get quantitative assessment of a repository. For these purposes, underground laboratories in the different geological formations have been constructed for extensive research covering geomechanical, geohydraulic, geochemical investigations of geological circumstances, geotechnical materials and their interaction.

In Europe, underground laboratories have been constructed in recent decades, e.g. Grimsel Test Site (Switzerland) and Hard Rock Laboratories Äspö (Sweden) in the granitic rock; Rock laboratories Mont Terri (Switzerland) and Bure (France) in clay rock. Different field experiments have been conducted for the understanding of processes under the in situ conditions. To implement experimental data gained from the in situ test, a multiple-process coupled code is required.

In the course of the quick development of computer technology, numerical codes with capability to analyze problems in the coupled manner have become possible. However, the understanding of the complicated coupled processes based on the experimental data available and implementation of the developed algorithm into the numerical codes are a major challenge for scientists, which require interdisciplinary cooperation and interactive procedures.

Quality management and controlling is nowadays a standard tool for production and development to ensure a high quality of a produced result. A numerical code dealing with the coupled THMC process is highly complicated software product, since the different processes have different characteristic features, e.g. time and spatial scales, nonlinearities, and interaction degree, etc. To keep the high quality of the developed code, benchmark testing is therefore necessary, especially in case scientists from different disciplinary and different organizations are working on the same code. Therefore, code verification and validation of selected test cases are documented, and finally a benchmarking book for code developers is produced and quality-ensured (*Kolditz et al.* [4])

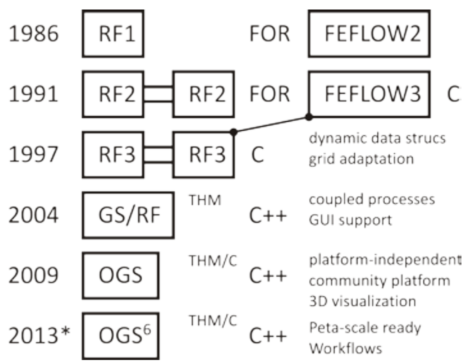


Figure 1: Code development history path

The modeling concept for thermo-hydro-mechanical-chemical processes in fractured-porous media has been developed continuously since the mid-Eighties (Fig. 1). As a merger of RockFlow and FEFLOW idea concerning multi-dimensional finite elements and dynamic data structures for grid adaptation purposes, OGS became an open source project since 2009 at the Helmholtz Centre for Environmental Research UFZ. Since last the development of the new version ogs6 started under GitHub https://github.com/ufz/ogs. The paradigms for ogs6 are: complete modeling work flows, developer and user-friendly, and ready for Peta-scale computer systems.

APPLICATION AREAS

Geotechnics

The coupling phenomena of thermal (T), hydraulic (H), and mechanical (M) processes are important for the analysis of deep geosystems under high temperature, pressure and stress conditions. Application areas of THM coupled models are e.g. geothermal energy utilization, nuclear waste disposal, and carbon dioxide storage in the deep geological formation.

The following slides illustrate that the understanding of THM processes, including chemical reactions (C process) is important to a large variety of geotechnical and geothermal applications. The physical basics are exactly the same for these applications. Different is simply

- the geological environment and different rock types, i.e. crystalline rocks, volcanic rocks, sandstones, clay, bentonite, ...
- the geofluids, i.e. water, brines, vapour, methane, carbon dioxide, ...
- the thermodynamic conditions, i.e. temperature, stress, pressure, salinity, …

There are several concepts concerning host rock for the disposal of hazardous waste in deep geological media, i.e. crystalline, salt, sediment, and volcanic formations. Different concepts use different buffer systems as geotechnical barriers for the waste isolation, i.e. crushed salt, bentonite, and bentonite/sand mixture. THM/C coupled modelling is required for the long-term analysis of possible processes which might result in a release of contaminants from the repository [106]. In that case it is important to know, how long it will take until the contaminants return into the biosphere.

Fig. 2 illustrates the application area: Carbon Capture Storage (CCS). The idea is to capture the CO2 from the power plants, liquefy it and inject it into the subsurface for long-term storage. Two basic concepts for appropriate geological systems are under proof now: depleted gas reservoirs and deep saline aquifers. After many years of operation many former gas reservoirs are depleted. These reservoirs are in an under-pressurized status and can take up large volumes of fluids. Keeping the reservoir under- pressurized and the impervious cap rocks are important considerations for storage. THM/C modelling is required in order to calculate the possible fluid storage capacity and to better understand the highly coupled processes in the CO2 injection area as well as their consequences for the storage concept (*Goerke et al.* [5]).

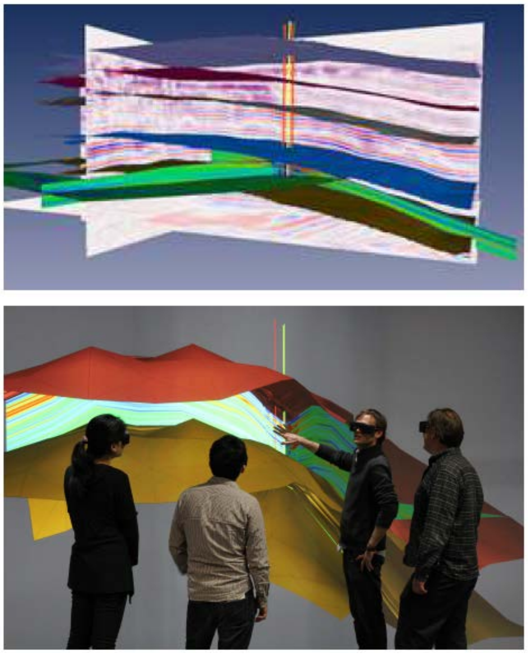


Figure 2: Data integration and modeling CO2 injection into the Ketzin test site which is operated by the GFZ (*Martens et al.* [6]). The upper figure shows the combination of structural geological information with geophysical data from seismic investigation. The lower figure depicts the facies information on permeability distribution in the saline aquifers. The 3D visualization is shown in the visualization center VISLAB of the UFZ (*Zehner* [7]).

Geothermal Energy

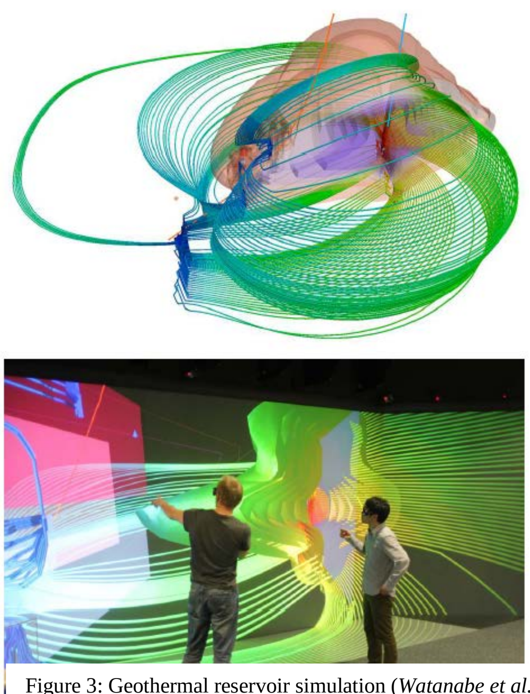


Fig. 3 depicts the application area: Geothermal energy, which is one of the alternative future energy resources under consideration. So-called shallow and deep geothermal systems are distinguished. Shallow systems are already commercially used e.g. for heating purposes. Deep geothermal reservoirs can be used for electric power production as high temperatures up to 200 C can be produced. THM/C modeling is required to design these geothermal power plants, e.g. in order to optimize production efficiency and reservoir lifetime. The significant cooling of the reservoir due to fluid reinjection gives rise to thermo-mechanical effects which need to be controlled in order to avoid reservoir damage.

Figure 3: Geothermal reservoir simulation (*Watanabe et al.* [8]). The upper figure shows the flow and heat transport OGS simulation of the geothermal test site Groß Schönebeck which is operated by the GFZ. The lower figure depicts the 3D visualization in the visualization center VISLAB of the UFZ (*Bilke et al.* [9]).

Hydrogeology

The second application area for coupled process simulation is hydrology. River basins or catchments are also subject to THMC coupled processes, but include however a completely different range of thermodynamic conditions than deep geological systems. Hydrological processes are very complex to describe as they vary highly in time and space. The evaluation of groundwater recharge is vital to a sustainable water resources management (so called safe yield). To this purpose, i.e. the understanding of small scale phenol-mena such as root / soil water interaction is of tremendous significance (*Kalbacher et al.* [10]). Typically groundwater models are used for management purposes particularly in semi-arid areas such as the Jordan Valley in the Middle East.

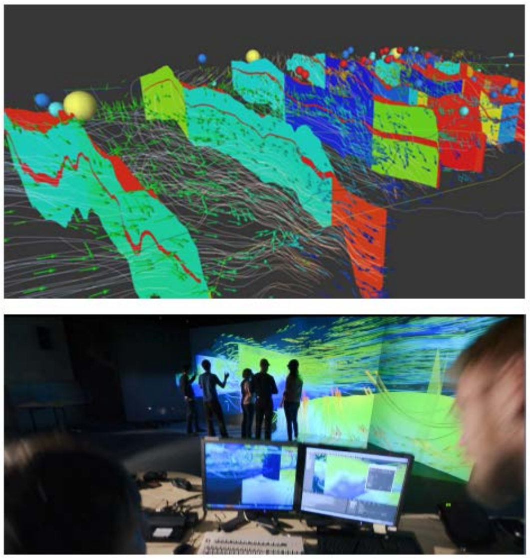


Figure 4: Groundwater simulation: The upper figure shows the OGS groundwater model for a catchment in the Jordan River valley (*Gräbe et al.* [11]). The lower figure depicts the 3D visualization of a river-hyporheic coupled system in the visualization center VISLAB of the UFZ (*Rink et al.* [3]).

Because water availability is an important issue in semi-arid and arid regions, groundwater quality deterioration is a critical concerning many urban areas of the world. Fig. 5 shows as an example part of a groundwater quality model prepared for the Nankou basin in the greater Beijing area. The idea of this modelling project is to identify possible sources of nitrate contamination originating from intense agriculture and fertilizer production (*Sun et al.* [12]). Land use and climate changes will impact the availability and quality of water resources to a large degree in the future. The modelling should help to develop scenarios for improving the groundwater quality in the long term. Areas subject to large groundwater extraction are also subject to severe land subsidence.

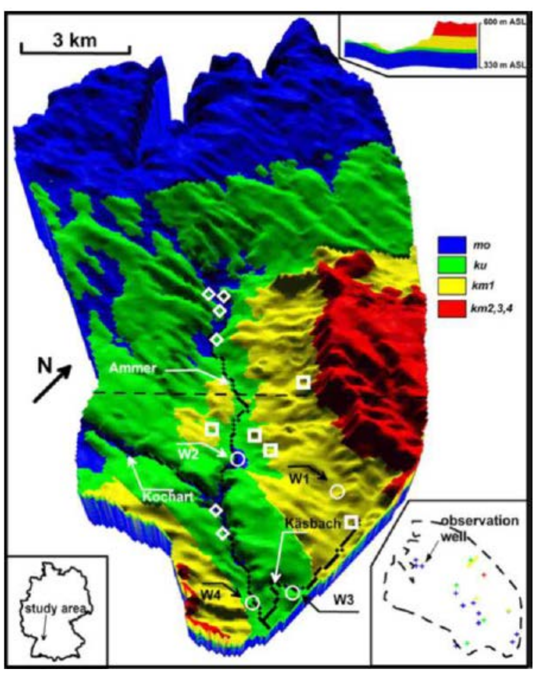
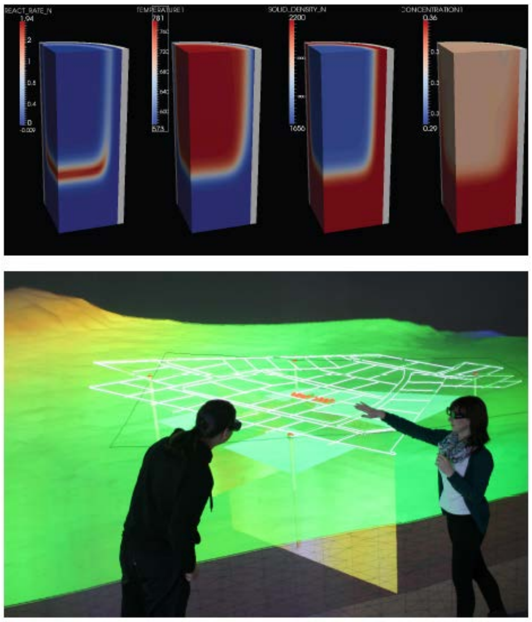


Figure 5: Groundwater model for the Ammer catchment (*Selle et al.* [13]).

Energy Storage



A very recent research area for THMC modelling has become energy storage. The economy and feasibility of renewable energy sources will depend a large degree on efficient energy storage systems. Fig. 6 shows the numerical simulation of flow and heat distribution in a solid thermal energy storage block, which will be used to store solar energy collected during the daytime for use at night (so called solar-thermics). The long term stability and efficiency of those energy storage devices can be optimized using THMC modelling (i.e. solving the inverse geothermal problem). In addition to thermal storage, thermo-chemical concepts are under development, i.e. storing thermal energy by triggering endothermic reactions and gaining thermal energy back on demand with the reverse reaction (exothermic).

Figure 6: Heat storage and extraction: The upper figure shows the OGS simulation for optimizing thermo-chemical heat storage (*Nagel et al.* [14]). The lower figure depicts the 3D visualization of a shallow geothermal test site in the visualization center VISLAB of the UFZ (*Schelenz et al.* [15]).

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The manuscript is based on the book introduction by *Kolditz et al.* [4]. For more information we refer to this forthcoming book publication and to the OGS community web page www.opengeosys.org.

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