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Open-source Python library for modeling coupled thermo-hydro-mechanical (THM) processes

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Abstract. The interactions between temperature, fluids, and mechanical properties in a repository system are essentially described scientifically by coupled thermo-hydro-mechanical (THM) processes. THM modeling, i.e., the prediction of the behavior of materials under different conditions, is the fundamental numerical tool here. The confident handling and deep understanding of numerical computation methods is thus the prerequisite for performing and evaluating preliminary safety analyses in the site selection process.

At the Federal Office for the Safety of Nuclear Waste Management (BASE), a software library for the simulation of coupled THM processes is currently being developed. The main goal of the in-house development is an open-source toolbox in the scripting language Python and is motivated by several long-term sub-goals:

- targeted development of expertise within BASE regarding numerical modeling of safety-relevant aspects in the long-term safety analyses;
- diversification of the testing capabilities regarding the preliminary safety investigations by means of an in-house, independent modeling software;
- foundation of a library of known benchmarks and evaluation examples for the comparison of different software tools;
- documentation and processing of basic THM scenarios for internal or, if necessary, public technical training.

The focus of this development is on creating a toolbox that is easy to use and at the same time highly flexible. The main methodical aspects are as follows:

- building a new library based on the pyGIMLi pre- and postprocessing framework (Rücker et al., 2017);
- creating a finite-element reference implementation in the Python scripting language for maximal transparency;
- creating an easy-to-use interface to the solution of the weak formulation for the finite-element theory with expressions of a symbolic manner allowing maximal flexibility;
- defining an interface to allow for the integration of alternative, third-party high-performance libraries;
- creating a collection of Jupyter notebooks of well-documented test cases and benchmarks.

Choosing the open-source approach ensures the best possible transparency and, in the long term, also allows the provision of appropriately quality-assured and documented simulation tools to the public. The presented poster shows the current development status of the software library and the currently implemented quality assurance concepts and gives an outline of the potential applications of the library.

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References

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