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OpenGeoSysUncertaintyQuantification.jl: a Julia library implementing an uncertainty quantification toolbox for OpenGeoSys

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Software

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Abstract

In the simulation-aided design of safety-related projects, the effects of uncertainties in the input parameters on the outcome are often of great interest. OpenGeoSys 6 (OGS6) is an open-source scientific project for simulating thermo-hydro-mechanical (THM) processes in porous media. Various parameters are needed for this kind of complex coupled simulation, many of which are subject to uncertainty due to imprecise knowledge. OpenGeoSysUncertaintyQuantification.jl is a Julia library that provides all the necessary global sensitivity analysis and uncertainty quantification methods in a validly configured deterministic OGS6 model.

Statement of need

Stability verifications for large structures can often only be carried out with the help of numerical simulations. A particularly difficult example is the safe storage of highly radioactive waste in subsurface repositories. These are usually planned at depths of several hundred meters. The heat radiated by the fuel rods can influence thermal-hydraulic-mechanical processes down to depths of several kilometers. Numerical simulations are needed to ensure site safety (Hoyer et al., 2021). Because of the outstanding interest in the safety of these repositories, the uncertainties are also given special attention (Kurgyis et al., 2024). OpenGeoSys is a frequently used simulation tool in the German research community dedicated to the containment-safe storage of radioactive waste. Due to legal requirements in the repository safety ordinance, it is necessary to quantify input uncertainties of a deterministic OGS6 model.

Parameterizing a THM model in OpenGeoSys (Kolditz et al., 2012) is complex and time-consuming due to the large number of possible input parameters. This package was designed with the aim to be explicitly related to the OGS6 project. However, care was taken to ensure that the underlying packages could potentially be still applicable to other projects.

For this toolbox, the following stochastic modeling strategy was chosen: the less known the effect of the input uncertainty on the output, the more general the quantity of interest should be selected. As a first step, selecting a complete OGS6 postprocessing result is a viable option. This approach provides methods to `explore` uncertainties in the OGS6 simulation output.

The OpenGeoSys community commonly uses Python; however, Julia was chosen for this project due to its superior efficiency and built-in capabilities for distributive computing.

To this date, there is no uncertainty quantification toolbox for OpenGeoSys, neither in Python nor in the Julia language. However, a general-purpose uncertainty quantification package named UncertaintyQuantification.jl is available for the Julia language.

Features

Most of the functionalities of this package are outsourced into independent Julia packages to maintain their generic character. Therefore, OpenGeoSysUncertaintyQuantification.jl serves as an umbrella project for the following projects:

- DistributedSparseGrids.jl (Bittens & Gates, 2023; Gates & Bittens, 2015)

  A library implementing an Adaptive Sparse Grid collocation method for integrating memory-heavy objects generated on distributed workers.

- DistributedMonteCarlo.jl

  A library implementing a Monte Carlo method for integrating memory-heavy objects generated on distributed workers.

- Ogs6InputFileHandler.jl

  A simple OGS6 input file handler.

- VTUFileHandler.jl (Bittens, 2022)

  A VTU library for reading and writing vtu files. In addition, all mathematical operators are provided needed for stochastic postprocessing. As a result, the datatype `VTUFile` can be used directly with the adaptive sparse grid or in a Monte Carlo analysis, enabling interpolation and integration for sets of OGS6 results.

- XDMFFileHandler.jl

  Analogous to the above, this is a file reader for the XDMF result file format. Provides the datatype `XDMF3File` compatible with stochastic postprocessing.

Features of OpenGeoSysUncertaintyQuantification.jl:

- Setup of stochastic OGS6 projects (see docs).
- Definition of input parameters and (truncated) input distributions via Distributions.jl (Lin et al., 2019).
- Adaptive sparse grid surrogate modeling of the physical state space. All snapshots have to fit into the system memory.
- Distributed Monte Carlo integration. Snapshots do not have to fit into the system memory collectively.
- Monte Carlo integrated Sobol' indices.
- Monte Carlo or Latin Hypercube integrated Morris means.
- Computation of expected value, variance, or sensitivity indices of complete OGS6 postprocessing results.

To enable the stochastic postprocessing of large data sets, special attention was paid to implement allocation-free in-place variants of all necessary math operators for all output datatypes such as a `VTUFile` or `XDMF3File`.

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