EGU21-2290
https://doi.org/10.5194/egusphere-egu21-2290
EGU General Assembly 2021


# An open-source integrated solution for flow and transport in random heterogeneous porous media

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Due to the increasing challenges to preserve water quality and supply at global scale, groundwater flow modeling has become a tool of pivotal relevance for remediation, implementation of policies, and design of applications for recharge management. The strain towards faster and more reliable hydrogeological simulations triggered the development of upscaled and multi-scale approaches employing different diffusion and dispersion models that are still the object of much debate in the community. Our ongoing study focuses on the up scaling of solute transport through heterogeneous geological domains by means of an extensive three-dimensional simulation study, based on a new open-source C++ library, built on top of the well-know finite-volume library OpenFOAM®. We integrate the whole workflow, from geostatistical random field generators to flow and transport solvers with integrated post-processing capabilities. The robustness, scalability and flexibility of the library makes it suitable framework for the development, testing, and application of upscaling techniques.

Being the subsurface inaccessible by nature, the appeal to geostatistical techniques is a well-established approach to construct a realistic domain for flow and transport simulations. However, additional challenges are posed by the numerical simulation of highly heterogeneous materials. Indeed, the problem is twofold: on one side it is not always possible to characterize the heterogeneity in a deterministic way, while on the other side numerical methods which are effective for elliptic and parabolic equations solved over homogeneous domains might suffer in heterogeneous media. Both challenges were effectively tackled using the open-soruce library OpenFOAM whose implementation and capabilities will be illustrated. Preliminary results on flow and transport simulations performed on truncated pluri-Gaussian permeability fields will be shown and the influence of geostatistical metrics (e.g. correlation lengths, variance, geological entropy) on the flow and transport results (e.g. average velocity and breakthrough curves) analysed.

Extensions to variable-density, mobile-immobile, and multi-rate mass transfer formulations are also presented in the context of the EU project “SECURe”.