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SHEMAT-Suite: a parallel open source simulator for flow, heat and mass transport in porous media

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We present SHEMAT-Suite, a numerical code for simulating flow, heat, and mass transport in porous media that has been published as an open source code recently. The functionality of SHEMAT-Suite comprises pure forward computation, deterministic Bayesian inversion, and stochastic Monte Carlo

simulation and data assimilation. Additionally, SHEMAT-Suite features a multi-level OpenMP parallelization. Along with the source code of the software, extensive documentation and a suite of test models is provided.

SHEMAT-Suite has a modular structure that makes it easy for users to adapt the code to their needs. Most importantly, there is an interface for defining the functional relationship between dynamic variables and subsurface parameters. Additionally, user-defined input and output can be implemented without interfering with the core of the code. Finally, at a deeper level, linear solvers and preconditioners can be added to the code.

We present studies that have made use of the code's HPC capabilities. SHEMAT-Suite has been applied to large-scale groundwater models for a wide range of purposes, including studying the formation of convection cells, assessing geothermal potential below an office building, or modeling submarine groundwater discharge since the last ice age. The modular structure of SHEMAT-Suite has also led to diverse applications, such as glacier modeling, simulation of borehole heat exchangers, or Optimal Experimental Design applied to the placing of geothermal boreholes.

Further, we present ongoing developments for improving the performance of SHEMAT-Suite, both by refactoring the source code and by interfacing SHEMAT-Suite with up-to-date HPC software. Examples of this include interfacing SHEMAT-Suite with the Portable Data Interface (PDI) for improved data management, interfacing SHEMAT-Suite with PetSC for MPI-parallel solvers, and interfacing SHEMAT-Suite with PDAF for parallel EnKF algorithms.

The goal for the open source SHEMAT-Suite is to provide a rigorously tested core code for flow, heat and transport simulation, Bayesian and stochastic inversion, while at the same time enabling a wide range of scientific research through straightforward user interaction.

