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Challenges in improving the HPC efficiency of the GEOtop 2.1 Integrated Hydrologic Model

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Integrated hydrological modeling systems simulate complex interactions between groundwater, surface water flows, vegetation and atmosphere under heterogeneous conditions. The mathematical representation of these interactions in simulation models is still a great challenge because of the composite physical processes described by a mixture of nonlinear, coupled partial differential equations and empirical representations. Therefore, the developed codes are often not easy portable and difficult to be handled. Moreover, the application of integrated hydrological models to large domains or long time series (i.e. climate research) requires significant computational efforts.
GEOtop is an open-source integrated model implemented in C/C++, published under GPL v3.0 license (http://geotopmodel.github.io/geotop/). It describes the three-dimensional water flow in the soil and the energy exchanges with the atmosphere, considering the radiative and turbulent fluxes. Furthermore, it reproduces the highly non-linear interactions between the water and energy balance during soil freezing and thawing, and simulates the temporal evolution of snow cover, soil temperature and moisture.
However, despite the number of research applications performed so far, the lack of a modern software engineering approach is hindering its further scientific development. Moreover, the lack of parallelization of the numerical solvers prevented its use over large domains or at high spatial resolution or the application of automatic sensitivity and optimization tools.
In this contribution we present our recent software re-engineering efforts to create a robust and computationally efficient scientific software package open to the hydrological community, easily usable by researchers and other experts.
A Continuous Integration mechanism by means of Travis-CI has been enabled on the github repository on master and main development branches. This system allows an efficient comparison and scientific validation over a certain number of referenced results as benchmark every time a software re-engineering activity is performed on the model. Benchmark tests have been selected from already published case studies in order to cover for different possible model configurations and target hydrological quantities (i.e. runoff, energy fluxes).
Model performances have been then analyzed for the benchmark simulations to identify model structural deficiencies and the parts of the code that limit model performance. Finally, code profiling results will be presented and discussed for the benchmark simulations. The final goal is to define an effective strategy to improve computational efficiency through minor changes/rearrangements in the code and partial parallelization.