A modern software approach to improve the computational efficiency of the integrated hydrological model GEOtop

Elisa Bortoli, OGS, National Institute of Oceanography and Applied Geophysics, Trieste, Italy
Giacomo Bertoldi, Institute for Alpine Environment, Eurac Research, Bolzano, Italy.
Samuel Senoner, ICT Department, Eurac Research, Italy.
Emanuele Cordano, Rendena100, Engineering and Consultancy sole proprietorship, Tione, Italy.
Matteo Camporese, University of Padova, Padova, Italy.
Stefano Cozzini, CNR/IOM, Trieste, Italy.

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Abstract

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 [1], 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 [2, 3] is an open-source integrated model implemented in C/C++. 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 a modern software engineering approach hindered its further scientific development without a huge amount of work and a deep knowledge of the detailed structure of the code. Moreover, the lack of a parallelization of the computing algorithms hindered 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 experts.

Our ultimate goal is twofold: from one side to strongly improve the usability of the package by the user community from the other side to improve the computational efficiency of the package.

To keep track of any single change the package has been published on its own github repository http://geotopmodel.github.io/geotop/ under GPL v3.0 license. 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 package. Benchmark tests have been selected form already published case studies in order to cover for different possible models 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 which limit models performances. Finally, a strategy to improve models computational efficiency trough minor changes/rearangements in the code and partial parallelization will be presented and evaluated for the benchmark simulations.

References