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# Coupling R and PHREEQC: an interactive and extensible environment for efficient programming of geochemical models

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PHREEQC [1] is a widely used non-interactive open source software for speciation, batch-reactions, one-dimensional transport, and inverse geochemical caclulations. It represents the tool of choice for many researchers and practicioners for a broad set of geochemical problems, underground $CO_2$ storage among others. Its open source nature, the flexibility to program arbitrary kinetic laws for the chemical reactions, as well as a thorough implementation of the Pitzer formalism explain its success and longevity. However, its non-interactive architecture make it cumbersome to couple PHREEQC to transport programs to achieve reactive transport simulations [2], but also to overcome the limitations of PHREEQC itself regarding the setup of large numbers of simulations - for example exploring wide ranges of conditions - and the graphical evaluation of the results. This has been the main motivation leading to the development of an interface with the high level language and environment for statistical computing and graphics GNU R [3].

The interface consists of minor modifications in PHREEQC's C source code, only affecting data I/O, plus on the R side a bunch of helper functions used to setup the simulations - basically automated manipulation of PHREEQC's input files, which are text files - and to collect and visualize the results. The most relevant subset of PHREEQC's capabilities and features are fully usable through the interface.

Illustratory examples for the utility of this programmable interface were given in the framework of the research project this developement originated from: CLEAN [4], a project investigating the feasibility of enhanced gas recovery combined with $CO_2$ storage. This interface allowed us to successfully and easily manipulate, compare and refit chemical databases, perform sensitivity analysis by combinatory variations of parameters, and all that in an environment which is both scriptable and interactive, with all results directly available for further manipulations and visualization in a powerful high level language, and benefiting from an enormous amount of third-party open source R extensions.

The possibility to rapidly prototype complex algorithms involving geochemical modelling is in our opinion a huge advantage. A demonstration is given by the successful evaluation of a strategy to reduce the CPU-time needed to perform reactive transport simulations in a sequential coupling scheme. The idea is the "reduction" of the number of actual chemical simulations to perform at every time step, by searching for "duplicates" of each chemical simulations in the grid: such comparison involves typically a huge number of elements (one chemical simulation for grid element for time step) and a quite large number of variables (concentrations and mineral abundances). However, through the straightforward implementation of the prototype algorithm through the R/PHREEQC interface, we found out that the scan is extremely cost-effective in terms of CPU-time and typically allows a relevant speedup for simulations starting from a homogeneous or zone-homogeneous state. This speedup can even greatly exceed that of parallelization in some favorable but not unfrequent case. This feature should therefore be implemented in reactive transport simulators.

References

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