Geophysical Research Abstracts
Vol. 17, EGU2015-9785, 2015
EGU General Assembly 2015

Reactive transport modeling in the subsurface environment with OGS-IPhreeqc

Wenkui He (1,2), Christof Beyer (3), Jan Fleckenstein (1), Eunseon Jang (1,2), Thomas Kalbacher (1), Dimitri Naumov (1), Haibing Shao (1,4), Wenqing Wang (1), Olaf Kolditz (1,2)

(1) Helmholtz Centre for Environmental Research, Environmental Informatics, Leipzig, Germany (wenkui.he@ufz.de), (2) Applied Environmental System Analysis, TU Dresden, Germany, (3) Institute of Geosciences, Geohydromodelling, Christian-Albrechts-University of Kiel, Germany, (4) Faculty of Geosciences, Geotechnics and Mining, Freiberg University of Mining and Technology, Germany

Worldwide, sustainable water resource management becomes an increasingly challenging task due to the growth of population and extensive applications of fertilizer in agriculture. Moreover, climate change causes further stresses to both water quantity and quality. Reactive transport modeling in the coupled soil-aquifer system is a viable approach to assess the impacts of different land use and groundwater exploitation scenarios on the water resources.

However, the application of this approach is usually limited in spatial scale and to simplified geochemical systems due to the huge computational expense involved. Such computational expense is not only caused by solving the high non-linearity of the initial boundary value problems of water flow in the unsaturated zone numerically with rather fine spatial and temporal discretization for the correct mass balance and numerical stability, but also by the intensive computational task of quantifying geochemical reactions.

In the present study, a flexible and efficient tool for large scale reactive transport modeling in variably saturated porous media and its applications are presented. The open source scientific software OpenGeoSys (OGS) is coupled with the IPhreeqc module of the geochemical solver PHREEQC. The new coupling approach makes full use of advantages from both codes: OGS provides a flexible choice of different numerical approaches for simulation of water flow in the vadose zone such as the pressure-based or mixed forms of Richards equation; whereas the IPhreeqc module leads to a simplification of data storage and its communication with OGS, which greatly facilitates the coupling and code updating. Moreover, a parallelization scheme with MPI (Message Passing Interface) is applied, in which the computational task of water flow and mass transport is partitioned through domain decomposition, whereas the efficient parallelization of geochemical reactions is achieved by smart allocation of computational workload over multiple compute nodes. The plausibility of the new coupling is verified by several benchmark tests. In addition, the efficiency of the new coupling approach is demonstrated by its application in a large scale scenario, in which the environmental fate of pesticides in a complex soil-aquifer system is studied.