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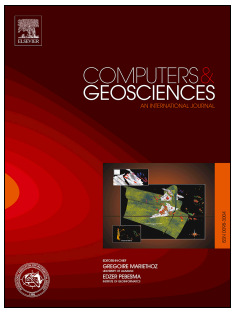

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Daniel Jara, Jean-Raynald de Dreuzy, Benoit Cochepin

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TReacLab: an object-oriented implementation of non-intrusive splitting methods to couple independent transport and geochemical software

Daniel Jara[1], Jean-Raynald de Dreuzy[1], Benoit Cochepin[2]

[1]Géosciences Rennes, UMR CNRS 6118, Campus de Beaulieu, University of Rennes 1, Rennes, France

[2]ANDRA, 1/7 Rue Jean Monnet, 92298 Châtenay-Malabry, France

Abstract

Reactive transport modeling contributes to understand geophysical and geochemical processes in subsurface environments. Operator splitting methods have been proposed as non-intrusive coupling techniques that optimize the use of existing chemistry and transport codes. In this spirit, we propose a coupler relying on external geochemical and transport codes with appropriate operator segmentation that enables possible developments of additional splitting methods. We provide an object-oriented implementation in TReacLab developed in the MATLAB environment in a free open source frame with an accessible repository. TReacLab contains classical coupling methods, template interfaces and calling functions for two classical transport and reactive software (PHREEQC and COMSOL). It is tested on four classical benchmarks with homogeneous and heterogeneous reactions at equilibrium or kinetically-controlled. We show that full decoupling to the implementation level has a cost in terms of accuracy compared to more integrated and optimized codes. Use of non-intrusive implementations like TReacLab are still justified for coupling independent transport and chemical software at a minimal development effort but should be systematically and carefully assessed.