High performance Computing for two-phase reactive flows in porous media

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Reactive multiphase multicomponent flows in porous media are involved in many applications related to subsurface environment and energy issues. Such flows are governed by a set of highly nonlinear system of degenerate partial differential equations (describing a multiphase compositional flow) coupled with algebraic and/or ordinary differential equations (related to geochemical model) requiring special numerical treatment. The numerical strategies for solving this system are divided into two categories : the global implicit and the sequential approaches. The global implicit approach solves one nonlinear system gathering all equations at each time step while for the sequential approach, flow and reactive transport are solved sequentially at each time step.

In the framework of the parallel platform DuMu^X [1], we have developed and implemented several finite volume schemes to tackle such problems. Firstly, we developed a sequential approach solving a two-phase compositional flow problem and then a reactive transport problem using a direct substitution approach (DSA) [2]. Both subsystems are discretized in a fully implicit manner. Nonetheless, sequential approaches can introduce operator splitting errors. By consequence, we developed and implemented a fully-coupled, fully implicit method to solve reactive two-phase flows to achieve improved stability [3]. Both strategies were validated by numerous test cases including High Performance Computing. An advanced comparison between both strategies for a three dimensional scenario of geological storage of CO_2 will be presented.

Références

[1] B. Flemisch, M. Darcis, K. Erbertseder, B. Faigle, A. Lauser, K. Mosthaf, S. Muthing S., P. Nuske, A. Tatomir, M. Wolf, and R. Helmig. DuMu^X : DUNE for multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media. Advances in Water Resources, Vol 3, 1102-1112, 2011.

[2] E. Ahusborde, B. Amaziane, M. El Ossmani, Improvement of numerical approximation of coupled two-phase multicomponent flow with reactive geochemical transport in porous media, Oil & Gas Science and Technology - Rev. IFP Energies nouvelles, Vol 73, 73, 2018.

[3] E. Ahusborde, B. Amaziane, M. El Ossmani, M. Id Moulay, Numerical modeling and simulation of fully coupled processes of reactive multiphase flow in porous media, Journal of Mathematical Study, Vol 52, 359-377, 2019.