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Simulation of reactive transport in heterogeneous porous media with a Newton-Krylov method

Tuesday, 31 May 2022 10:30 (15 minutes)

Reactive transport modeling in porous media involves the simulation of several physical and chemical processes: flow of fluid phases, transport of species and chemical reactions between species. After discretization, one obtains a highly nonlinear system of partial differential for transport, coupled to algebraic equations for chemistry.

In [1], we have presented a globally coupled approach, where transport and chemistry are solved in a fully coupled manner, while transport and chemistry modules are kept separate. The method uses the same fixed point formulation than the Standard Iterative Approach, but, at each time step the nonlinear system of algebraic equations that couples all chemical species at all mesh points is solved by a Newton-Krylov method. The linear system at each Newton step is solved by the GMRES method, with a Jacobian free implementation where the required matrix by vector product may be approximated by a finite difference quotient or computed exactly.

Linear and nonlinear preconditioners must respect the block structure of the system in order to remain matrix-free. We have shown that block Gauss-Seidel preconditioners is closely related to a non-linear elimination method, and that both give a method where the number of both Newton and GMRES iterations do not grow when the mesh is refined [2].

In this talk, we recall the main features of the method, and we present an extension to handle mineral precipitation and dissolution reactions using an interior point Newton method [3]. We also study the performance of the method on 2D heterogeneous geometries.

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References

Laila Amir, Michel Kern, “A global method for coupling transport with chemistry in heterogeneous porous media”, Computat. Geosci., 14 :465–481, 2010.

Laila Amir, Michel Kern, “Preconditioning a coupled model for reactive transport in porous media”, Int. J. Numer. Anal. Model., 16(1) :18–48, 2019.

Laila Amir, Michel Kern, “Jacobian free methods for coupling transport with chemistry in heterogenous porous media”, Water (13), 370, 2021.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Unsure

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