CEMRACS '08

Modelling and Numerical Simulation of Complex Fluids
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Simulation of reactive transport in porous media

Project proposed by

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Chemical phenomena play an important role in several situations in porous media simulations : alkaline perturbation at the clay - cement interface close to a geological nuclear waste storage site or CO2 sequestration studies. The reactivity of chemical elements has a direct influence on their time of residence in the subsurface. Properly simulating the evolution of chemical species in a porous medium requires an integrated model, including both chemical and transport phenomena.

In these simulations, one aims at describing how a set of chemical species interact between themselves and with the host rock, while being subject to transport and diffusion by the underlying flow.

Mathematically, one deals with a set of advection-diffusion PDEs coupled to algebraic equations (assuming chemical equilibrium). The resulting discrete problem, couples all chemical species at all grid points, and requires efficient solution techniques. In the past, these systems have been solved by a two-step "operator splitting" approach (more properly seen as a block Gauss-Seidel method), where transport and chemistry are solved for iteratively. This has the additional advantage that the coupling can be done without having to modify the transport and chemistry simulation codes, as they will typically have been developed by different teams.

For more difficult problems, this approach may overly restrict the time step in order to ensure convergence. Techniques based on Newton's method have better convergence properties, but require that the Jacobian matrix be stored and factored. For realistic problems involving a large number of chemical species, this may be impractical. The Newton--Krylov (Keyes and Knoll, 2004) method has emerged as a powerful way to solve non-linear problem without factoring, or even forming, the Jacobian matrix: the linear system at each Newton iteration is solved by a Krylov subspace method (usually GMRES), which only requires the ability to multiply the Jacobian by a vector, that is to compute a directional derivative. The convergence rate is as fast as that of Newton's method, but the method can be implemented in in unobtrusive way.

Experience with 1D systems has shown promising results on several test problems, and the goal of this project is to extend these results to 2D situations.

This project is part of the ANR project "High Performance Simulation of CO2 Sequestration", involving IFP, BRGM, INRIA, Ecole des Mines de St Etienne, and LAGA (Paris 13).