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GLOBAL METHOD FOR COUPLING REACTIVE TRANSPORT

*** Caroline de Dieuleveult[1], Jocelyne Erhel[2]**

[1] ANDRA
IRISA Campus de Beaulieu
35042 Rennes Cedex France
Caroline.de_Dieuleveult@irisa.fr

[2] INRIA
IRISA Campus de Beaulieu
35042 Rennes Cedex France
Jocelyne.Erhel@irisa.fr

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ABSTRACT

Understanding the evolution of underground radioactive waste storage is a very important but difficult issue. Among the different phenomena involved in this problem, we focus on chemistry and transport which have a great impact in the field close to the waste storage. Transport and chemistry are strongly coupled phenomena involving a system of nonlinear partial differential algebraic equations (PDAE).

A lot of approaches have been developed in order to simulate this problem. These approaches are based on different models or on different numerical methods. In this study, we consider three types of methods. The first method, used in the Phreeqc solver, is a non iterative split operator method which solves, for each time step, the advection transport, the chemical system, then the diffusive transport and again the chemical system. The second method, the sequential iterative approach (SIA), also solves separately chemistry and transport but simultaneously advection and diffusion. Finally, we consider our approach which is a global approach consisting in solving the whole reactive transport system. Until recently, global methods have been set aside because of higth memory requirements [5] but this have changed recently because of the increase in memory resources [1,2,3]. This motivates our interest in global method.

Our global method is based on the method of lines, which is a general procedure for solving partial differential equations. The idea is to discretise the system firstly in space, then in time. The goal of this approach is to use efficient and robust DAE solvers. Once we get a system of differential algebraic equations (DAE), we use the IDA library in the SUNDIALS package from Livermore National Laboratory. We have modified this solver in order to introduce the sparse linear solver UMFPACK.

We have implemented and validated our method with different test cases and more specially with an example described in the manual of Phreeqc [4]. This test case consists in a 1D column containing initially a solution of cations in equilibrium with a cation exchanger. A different solution is injected on top of the column. Different transport conditions have been applied to this column : advective-diffusive transport, pure advective transport and pure diffusive transport.

We obtain the same results with the three different methods. The two figures presented here concern advective-diffusive transport conditions. We show, on the first figure, the evolution of the CPU time in function of the number of cells in the mesh. Our method is the most efficient concerning CPU time when

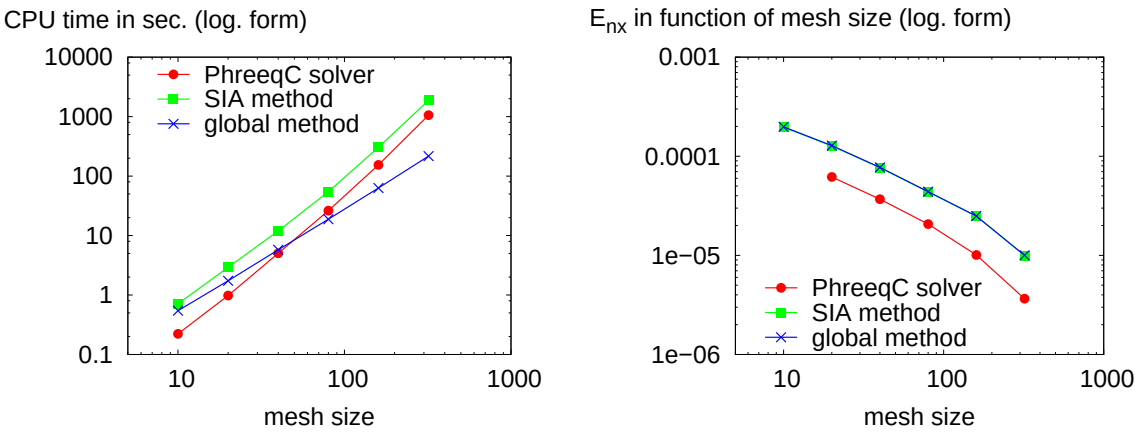

Figure 1: Evolution of the CPU time and evolution of E_{nx} in function of the mesh size nx. E_{nx} is the difference in L2 norm with concentrations having the finest mesh size nx_{max}, $E_{nx} = \sqrt{\frac{\sum_{j=1}^{n} |c_j^{nx} - c_j^{nxmax}|^2}{n}}$. n is the number of points of measure.

increasing the mesh size because of a lower slope. In the second figure, we present data related to the evolution of the concentration in function of the time at the end of the column for different values of the mesh size. As we do not have experimental or analytical evaluation of the solution, the reference is the concentration relative to the finest mesh, here equal to 640 mesh cells. The curves related to the three methods have the same slope. But the Phreeqc method is slightly more accurate than the two others methods.

Other test cases show that Phreeqc is well adapted to advective transport whereas the global method is efficient for diffusive one. In all our experiments, SIA is less or as accurate and requires more CPU time than our global method. Therefore, except for the advective case, our global method is the best method of the three regarding efficiency and accuracy.

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