

**Proposal for a trainee position in the French Nuclear Agency (CEA) in the Laboratory
for Flow and Transport Simulation for a student finishing the master's degree**

Domain : Numerical analysis

Duration : 6 months

Place : CEA-Saclay (parisian region, France)

Language: French or English or German

Contact : nikos.leterrier@cea.fr

Financial conditions: 700 euros/month gross (around 550 euros/month net), possible accomodation allowance around 220 euros/month and a bonus at the end of the internship.

We aim to test numerically a method for the analytical evaluation of the jacobian within the frame of resolving a coupled reactive transport system through Newton's or Non-Linear Conjugate Gradient methods. Reactive transport problems appear in many industrial areas such as the pollution studies or underground storage of nuclear waste, the latter being of interest here.

When chemical reactions are taken at thermodynamic equilibrium, it is impossible to write explicitly the chemical source terms in the reactive species' equations of evolution. It is fairly common to use an operator-splitting technique for sequential approaches and the direct substitution for a global approach. In both cases the jacobian is very often evaluated through a numerical approximation.

We aim here to evaluate the jacobian through an analytic calculation, using the mathematical properties of the chemical system (action mass laws), in the mainframe of a global approach, but without direct substitution. This analytical calculation is possible although the analytical expression of the function whose jacobian is calculated is unavailable.

The work will consist in proposing reactive transport tests in order to test this new method, and to compare the results with the numerical evaluation of the jacobian, and another analytical evaluation of the jacobian in the mainframe of the direct substitution approach. The accuracy of results and performances should be taken into account for this comparison. The trainee will be left free to choose the numerical tool for programmation: it can be C, C++ , Fortran etc...