Postdoctoral position: implementation of a software coupling tool for multi-physics problems

The increasing availability of open-source simulation codes facilitates the creation of multi-physics applications by means of a coupling tool capable of managing information transfers between codes in order to set up a coupling scheme adapted to the physical phenomena to simulate.
In the simulation of multi-physics applications, computing time is a major issue and requires the use of high-performance computing. The coupling algorithm is based on the exchange and processing of information between two or more parallel codes, each one using its own calculation grid, algorithms and temporal discretization adapted to the physical phenomenon to simulate.
Information transfers must be designed to maintain the code scalability and to preserve numerical precision. The transfer of data from one distributed interface to another one over a very large number of computing cores is a major challenge and existing solutions are not yet optimal.
In the context of geomechanical simulations, a proof of concept of coupling between a mechanical simulation code and a porous media flow simulation code has been implemented at IFPEN. After an analysis of the existing coupled code, the postdoctoral fellow will develop a new coupling tool in order to increase the performance of the existing coupled code, to improve its robustness and, possibly, its scalability:

- the data exchange strategy adopted by the existing coupled code is based on files, often originating significant latencies on data transfers. The postdoctoral fellow will overcome this limitation by implementing a new coupling tool based on a modern coupling technology. This development should also make it possible to better isolate the coupling interface between codes and make it more easily scalable.
- The sequential master-slave coupling scheme currently in place in the existing coupled code offers only a low degree of parallel scalability. The postdoctoral fellow will propose a solution to increase the parallel performance of the coupled code on modern architectures. The real difficulty of this challenge is the fact that it will not be possible to increase parallel performance by exploiting features available in the coupling interface without modifying the coupled codes. Indeed modifications of the coupled codes are expected to be very intrusive. The postdoctoral fellow will study a new coupling algorithm adapted to parallel decomposition. This new algorithm must be able to reproduce the results of the existing coupled code in a robust way. The postdoctoral fellow will probably need to modify the communication scheme between the coupled codes and to replace the fixed point method used in the existing coupled code.

Research program:

- study of existing coupling libraries (e.g.: CWIPI, Padawan, Precice) in order to be able to select the most suitable one for the new coupling tool ;
- study of the existing coupling tool and of the coupled codes, analysis of the physics of the coupled phenomena;
- selection of the coupling library to use for the new coupling tool;
- realization of a POC for the defined use case:
    - geomechanical coupling between a flow code in a porous medium and a mechanical simulator, such as Code_Aster.
- study of the implementation of a direct communication scheme replacing the centralized one used in the existing coupling tool;
- study of the possibility to use more efficient iterative coupling algorithms for non-linear problems by replacing the fixed point algorithm currently used in the existing coupled code.

Required skills: knowledge of C/C++, Fortran 90/2003, Python, numerical analysis, code coupling, Linux
Duration: 12 months
Simulation environment: IFPEN Linux HPC cluster
Supervision: multidisciplinary teams with mathematical, physical and computer skills.

Location: IFPEN (Rueil-Malmaison) and Andra (Chatenay-Malabry)

Contact: Bernard Vialay: Bernard.Vialay@andra.fr, Daniele Colombo: daniele.colombo@ifpen.fr and Ani Anciaux-Sedrakian: ani.anciaux-sedrakian@ifpen.fr