Iterative coupling algorithms and nonlinear solvers for the simulation of Thermo-Hydro-Mechanical models in faulted geological systems.

Coupled Thermo-Hydro-Mechanical (THM) processes in faulted/fractured geological systems play a fundamental role in many geoscience applications such as geothermal energy and geological storage. This is particularly the case in the field of CO2 sequestration where the pressurized, low-temperature injection of supercritical CO2 is likely to induce a reactivation of faults leading to risks of leakage and/or seismicity which must be mitigated. Numerical simulation is a key tool for better assessing and controlling these risks. Such models couple non-isothermal multiphase flows along the fault network and in the surrounding rock (the matrix), the rock mechanical deformation and the mechanical behavior of the faults. Their numerical simulation raises numerous challenges related to the complexity of the geometries, the heterogeneous and multi-scale properties characteristic of geological systems and the multi-physics and non-linear couplings.

The project focuses on the design of robust nonlinear solvers which constitutes a bottleneck for the simulation of these models. There are three types of approach to solve these coupled processes. The first, often referred to as monolithic, is based on solving simultaneously all equations by a Newton algorithm. It lacks modularity and requires a robust preconditioner for the linearized coupled system, which constitutes a difficult task subject of ongoing research. It also has the disadvantage of solving all the variables at the same time step, preventing the use of smaller time steps for the time integration of the multiphase flow.

On the other hand, time splitting algorithms, decoupling the thermo-hydro from the mechanical sub-models, make it possible to adopt such a sub-time step strategy for the flow. They rely on additional stabilization terms leading to either Fixed-Stress [2,7] or Undrained-Split [1] type splitting. However, these algorithms lack robustness in the incompressible limit and suffer from a loss of accuracy during regime changes and in case of strong hydromechanical couplings.

A good compromise is based on the iterative variant of the previous time splitting algorithms. Such algorithm iteratively solves the thermo-hydro and mechanical sub-models until convergence towards the coupled solution. Compared with the monolithic approach, it is more modular, allows the use of preconditioners adapted to each sub-model and the use of sub-time steps for the flow. Furthermore, their potential lack of robustness can be overcome by the use of acceleration techniques such as Newton Krylov [8,3], Conjugate Gradient [6] or Anderson [4,5] algorithms.

The first objective of the project is to explore iterative coupling algorithms and their acceleration techniques for THM models. Emphasis will be placed on the case of fractured/faulted models taking contact into account, which, to our knowledge, has not been yet investigated. A second aspect of the project concerns nonlinear solvers for the contact mechanics sub-model, which is particularly difficult in the case of stick-slip transitions due to the singularity of the friction laws [9,10].

Profile: applicants should have a background in scientific computing/numerical analysis/applied mathematics, and be familiar with the discretization of PDEs and iterative solvers. An experience in computational mechanics will be an additional asset.

Context: this position is a collaboration between Inria, University Côte d'Azur (Roland Masson and Konstantin Brenner) and IFPEN (Isabelle Faille and Guillaume Enchery) in the framework of the Inria-IFPEN partnership and of the project MathSout of the PEPR MathVives.

Location: the position will be held at the Laboratoire de Mathématiques J.A. Dieudonné (LJAD), Université Côte d'Azur, Nice, with regular visits at IFPEN, Rueil Malmaison.

Duration and starting date: the position is for two years and should start between September 2024 and the end of 2024.

Salary: About 2150 Euros net/month How to apply: send applications with CV, letter of motivation, and references, to <u>roland.masson@univ-cotedazur.fr</u>, <u>isabelle.faille@ifpen.fr</u> and <u>Guillaume.enchery@ifpen.fr</u>

Key words: scientific computing, coupled systems of PDEs, iterative coupling algorithms, nonlinear solvers, contact-mechanics, coupled thermo-poro-mechanical processes.

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