Position in scientific computing
High performance simulation of THM models in faulted geological systems
ANR project EARTH-BEAT

in collaboration between
BRGM
and
Université Cote d'Azur, Laboratoire de Mathématiques J.A. Dieudonné

February 9, 2024

Context

Thermo-Hydro-Mechanical (THM) models in faulted porous media play an important role in many applications in geosciences. Fault networks act as corridors for fluid flows and associated mass and energy transfers and they have a preeminent role on stress (re)distribution interacting with these transfers.

Anthropogenic exploitation of the subsurface (reinjection of geothermal brines, CO_2 sequestration...) can lead to pressure build-ups that can potentially lead to fault reactivation with induced seismicity and/or loss of storage integrity. Reciprocally, natural stress distribution in fault networks will constrain the pathways of hot geothermal brines and the location of associated geothermal resources and ore resources that they may have deposited.

Numerical modelling is a key tool to better understand, assess and control these processes. They couple the flow and energy transport along the faults and in the surrounding porous

Figure 1: Normal faults in volcanic ashes and paleo-soils, El Salvador, photo by Chuck DeMets

rock, the rock mechanical deformation, and the mechanical behavior of the faults related to contact-mechanics [1].

Among available numerical tools, ComPASS (https://gitlab.com/compass) is an open source parallel code initiated by LJAD-Inria and BRGM (Bureau de Recherches Géologiques et Minières - French Geological Survey) in 2015 [3, 4, 6, 5]. It is devoted to the simulation of multicomponent multiphase non-isothermal Darcy flows on polyhedral meshes and includes complex network of faults represented as interfaces of co-dimension one coupled to the surrounding matrix.

Understanding the genesis of ore deposition around fault networks is the topic of the EARTH-BEAT ANR project funding this position with a special focus on uranium deposits.

Work description

Main objectives

The objectives of the project are

(1) to developp in ComPASS a parallel 3D Thermo-Hydro-Mechanical numerical model adapted to polyhedral meshes and accounting for a linear elastic rock behavior with small deformations and frictional contact at matrix-fault interfaces,

(2) to couple this new contact-mechanical module with the multiphase non-isothermal flow model already implemented in ComPASS based on a robust iterative coupling strategy.

Provisional program

The choice of the discretization for the contact-mechanics adapted to polyhedral meshes and taking fault networks into account is a key point. It will be based on a mixed fomulation with face-wise constant Lagrange Multipliers accounting for the contact surface tractions at the matrix-fault interfaces. This choice allows to cope with fault networks including corners, tips and intersections and leads to local to each fault face contact conditions that can be solved with efficient semi-smooth Newton nonlinear solvers.

The discretization of the displacement field will be based on a low order Virtual Element Method (VEM) with nodal unknowns taking into account the discontinuity of the displacement field at matrix-fault interfaces. VEM is a natural extension of the $\mathbb{P}_1$ Finite Element Method (FEM) to polyhedral meshes. Its combination with a face-wise constant approximation of the Lagrange multiplier requires a stabilisation which will be achieved by enrichment of the displacement field with an additional "virtual" bubble unknown at one side of each fault face [2].

The solution of the sparse Jacobian system at each Newton iteration of the contact-mechanical model requires the implementation of an efficient parallel linear solver, typically using the Petsc library already available in ComPASS. In a first step, we will use a parallel direct sparse linear solver but iterative algorithms with on the shelves preconditioners could also be investigated in order to improve the efficiency of the simulations on realistic 3D geological models.

The coupling of the contact-mechanical and the non-isothermal multiphase flow models will be based on an iterative coupling strategy solving iteratively both nonlinear sub-problems until convergence up to a stopping criteria. The algorithm will be typically based on a fixed-stress [7] or undrained-split [8] fixed point method adapted to mixed-dimensional models and designed in order to allow for the use of smaller time steps for the flow model time integration. A possible acceleration of the fixed point algorithm could also be investigated in order to obtain a more robust convergence [9].

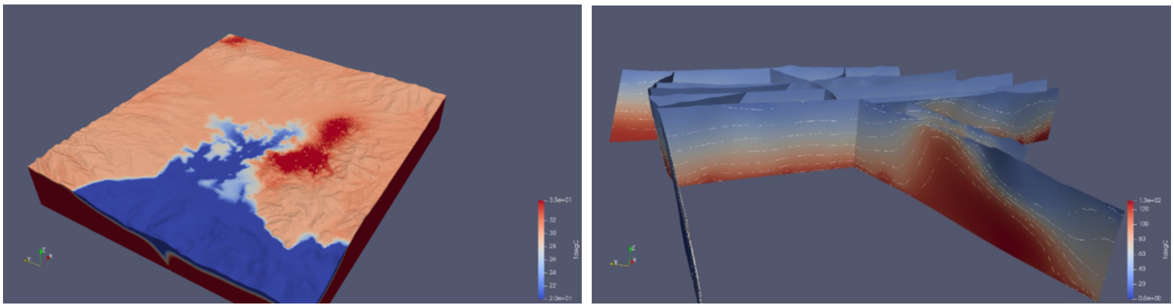

Figure 2: Simulation of the Baie du Lamentin hydrothermal system using ComPASS (Y. Labeau, Ph.D Thesis, 2018).

The developpment will be tested over reference tests and over more realistic applications comming from the EARTH-BEAT project partners.

Collaborations

This post-doctoral project is part of the ANR PRCE EARTH-BEAT 2024-2028 "Transient Thermo-Hydro-Mechanical couplings in hydrothermal systems - application to geothermal energy and giant mineral resources" in collaboration between GeoRessources/Université de Lorraine, BRGM, LJAD/UniCA, Mines Paris, LMV/Université Clermond Auvergne and Orano.

The post-doctoral work will be part EARTH-BEAT Work-Package 3 with the objective to implement in ComPASS a THM model in collaboration between Laurence Beaude, Simon Lopez, Farid Smai and Théophile Guillon from BRGM, and Roland Masson and Mohamed Laaziri from LJAD.

Position and application details

Profile: applicants should have a background in scientific computing/applied mathematics and be familiar with scientific programming (C++, Python, MPI) and collaborative development tools.

Location: the position will be held in BRGM, Orléans in association with the Laboratoire de Mathématiques J.A. Dieudonné (LJAD), Université Côte d'Azur. Several stays in LJAD are planned during the project.

Duration and starting date: the position is for two years and should start before the end of 2024 (ideally september 2024).

Salary: About 2200 Euros net/month

How to apply: send applications with CV, letter of motivation, and references, to
l.beaude@brgm.fr, t.guillon@brgm.fr, s.lopez@brgm.fr and roland.masson@univ-cotedazur.fr

Key words: scientific computing, high performance computing, virtual element methods, iterative coupling algorithms, contact-mechanics, hydrothermal fault systems, coupled thermo-poro-mechanical processes.

References

[1] F. Bonaldi, J. Droniou, R. Masson, A. Pasteau, Energy stable discretization of two-phase flow in deformable porous media with frictional contact at matrix-fracture interfaces, Journal of Computational Physics, January 2022. https://hal.archives-ouvertes.fr/hal-03349229

[2] J. Droniou, G. Enchery, A. Haidar, I. Faille , R. Masson, A bubble VEM-fully discrete polytopal scheme for mixed-dimensional poromechanics with frictional contact at matrix fracture interfaces, preprint december 2023, https://hal.archives-ouvertes.fr/hal-04343287v1

[3] F. Xing, R. Masson, S. Lopez, Parallel numerical modeling of hybrid-dimensional compositional non-isothermal Darcy flows in fractured porous media, Journal of Computational Physics, 345, pp. 637-664, 2017, https://hal.archives-ouvertes.fr/hal-01420361

[4] S. Lopez, R. Masson, F. Xing, L. Beaude, N. Birgle, F. Smai, K. Brenner, M. Kern, G. Courrioux, S. Caritg, Y. Labeau, Geothermal Modeling in Complex Geological Systems with the ComPASS Code. Stanford Geothermal workshop, February 12sd-14th 2018.

[5] Armandine Les Landes A., Beaude L., Castanon Quiroz D., Jeannin L., Lopez S., Smaï F., Guillon T., and Masson R. Geothermal Modeling in Complex Geological Systems with ComPASS, https://brgm.hal.science/hal-04246471, 2023.

[6] Antoine Armandine Les Landes, Daniel Castanon Quiroz, Laurent Jeannin, Simon Lopez, Roland Masson. Two-phase geothermal model with fracture network and multi-branch wells. The SMAI Journal of computational mathematics, Volume 9 (2023), pp. 121-149. https://smai-jcm.centre-mersenne.org/articles/10.5802/smai-jcm.97

[7] V. Girault, K. Kumar, and M. F. Wheeler. Convergence of iterative coupling of geomechanics with flow in a fractured poroelastic medium. Computational Geosciences, 20 (5), 997-101, 2016.

[8] T. Almani, K. Kumar, Convergence of single rate and multirate undrained split iterative schemes for a fractured Biot model, Computational Geosciences, 6, pp. 975-994, 2022.

[9] J. W. Both, K. Kumar, J. M. Nordbotten, F. A. Radu, Anderson accelerated fixed-stress splitting schemes for consolidation of unsaturated porous media, Computers and Mathematics with Applications 77 (6) (2019) 1479 - 1502.