

Joint Ph.D. position at the University of Lorraine (France) GeoRessources Laboratory / Laboratoire Magmas et Volcans (LMV) Title : Thermo-Hydro-Mechanical modeling of fault-valve behavior using a DEM approach

Context: Fault zones have complex internal structures in relation to host rocks, tectonic events and geological history. A convenient description which captures the main features of fault zones distinguishes the fault core (i.e., non cohesive cataclistic rocks such as fault breccia and fault gouge) and the damaged zone (fractured rocks containing subsidiary faults, fractures, fault-related folds and veins). Due to their structure, faults play a key role for subsurface flows, either in terms of sealing potential or in terms of flow channelization. Field observations suggest that some faults may act as valves in relation with tectonic events, promoting cyclic fluctuations in fluid pressure from supralithostatic to hydrostatic values. The reactivation of a fault, as a result of the coupling between fault slip and fluid overpressure, promotes flow discharge along the fault, which, in turn, leads to a lowering of the fluid pressure. The subsequent increase of the effective stress combined with hydrothermal self-sealing leads again to the reaccumulation of fluid pressure and thus to a repetition of the cycle. Such fault-valve behavior could play a key role in geothermal deposits and formation of hydrothermal ore deposits, whatever metal and age considered (Marz et al., 2019). Indeed, the heterogeneity of metal distribution observed for some ore deposits, such as the basement in the Athabasca Basin (Canada) for instance, suggests highly localized fluid circulations driven by anisotropy and spatial variation of permeability, mainly controlled by the properties and structure of faults. A similar behavior is observed for active geothermal systems. In addition, if fluid overpressure is considered one of the primary mechanisms that facilitate fault slip, other processes, such as thermal pressurization, might also trigger pore pressure increases in faults leading to their reactivation and to permeability changes.

Objectives and work summary: The complex evolution of fault permeability and strength during and after fault reactivation calls for a better description of the physical processes at stake. The current state-of-the-art in fault reactivation modeling proposes to describe macroscopically these weakening and strengthening mechanisms through phenomenological laws such as the widely used rate-and-state law. However, if these formulations have proven successful in reproducing some observed fault behaviors (e.g. Cappa and Rutqvist, 2011), they are based on empirically determined parameters and a part of the physics remain badly described (e.g., temperature effects, strain localization, permeability evolution associated to healing and sealing effects).



Figure 1. Numerical simulations of fluid pressurization of a granular shear zone by Nguyen et al (2021)

In this PhD thesis, we propose to relate the macroscopic response of both the gouge and damage zone of a fault to the micromechanical phenomena at work during its reactivation following the work initiated by Nguyen et al. (2021) and Zhang et al. (2021). For that purpose, we will utilize a discrete element model (DEM) coupled with a pore-scale finite volume (PFV) scheme implemented in the YADE DEM software (e.g., Mostafa et al., 2023). In a first step, we will simulate the steady state and transient behaviors of a sheared granular gouge under the effect of mechanical and hydraulic loadings (Figure 1), focusing more specifically on permeability evolution during the earthquake cycle simulated through the stick-slip dynamics of the modeled gouge. Then, we will examine the role of temperature on the overall behavior by considering either (or both!) the influence of thermal pressurization and shear heating. A similar investigation will be conducted for the damage zone. For that purpose, a discrete fracture network (DFN) will be generated and the hydraulic and mechanical responses induced by fluid overpressures will be simulated using a DEM model, either YADE DEM, or the 3DEC commercial software.

In a second step, we will pursue the goal of upscaling the micromechanical properties of the simulated media (the gouge and the damage zone) to determine the effective properties of faults, taking advantage from direct numerical simulations. Indeed, rather simple constitutive models are classically implemented to work at basin scale whereas behavior laws play a key-role in the HM response of faults to valving processes. Compressive and direct shear tests will be performed numerically under different confinement pressures and at different damage states to estimate both elastic and strength properties of faults. In a similar way, effective thermal conductivity and permeability will be derived respectively from heat conduction tests and fluid injection tests. A damage-dependent hydraulic aperture will be also derived and related to the fault permeability. Finally, these THM properties will be assigned to a simplified fracture model using the discrete element-based commercial software 3DEC for validation purpose. Advanced behavior laws will be studied in 3DEC, derived from upscaling and compared with pore-scale DEM simulations.

Student profile: The candidate must be a highly-motivated and self-directed person with a recent university master's degree (or equivalent) in computational mechanics, reservoir engineering, applied mathematics, civil engineering, or other relevant fields. He or she may demonstrate fundamental knowledge of solid and fluid mechanics principles governing the behaviour of porous and fractured media and motivation for work at the interface between disciplines. An experience in developing numerical methods, particularly DFN/DEM would be an asset, as well as knowledge of C++ and/or Python programming languages. Also, the candidate will need to be fluent in English.

Funding: The proposed PhD is funded as a part of the ANR research project EARTH-BEAT. This project, in collaboration with Orano Mining, BRGM, LJAD, Mines ParisTech, LMV and GeoRessources has the objective of boosting our understanding of mineral and geothermal resources and the development of predictive tools for potential assessment of these energy sources. This PhD is funded for 3 years, starting on October, 1st 2024 (gross salary, including social security: ~ 2 192 \notin /month).

Location: This full-time position will be shared between GeoRessources (Univ. Lorraine) and LMV laboratories (Univ. Clermont Auvergne). This joint PhD will be located in both institutions (Clermont-Ferrand/Nancy: 1.5 year each).

How to apply: Applicants should send via email a Curriculum Vitae, copy of the master thesis and the names and email addresses of two references to:

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References: Martz P., Mercadier J., Cathelineau M. ...& Ledru, P. (2019). Chem. Geology, 508, 116-143. /<u>10.1016/j.chemgeo.2018.05.042</u>; Cappa, F., Rutqvist, J., 2011. Int. J. Greenhouse Gas Control 5, 336–346. doi:10.1016/j.ijggc.2010.08.005; Nguyen H., Scholtès L., Guglielmi Y., Donzé F.V., Ouraga Z. et al., GRL 2020. <u>https:/dx.doi.org/10.1029/2021GL093222</u>; Zhang L., Scholtès L., Donzé F.V. (2021), Rock Mech. Rock Engng. 54, 6351-6372 <u>10.1007/s00603-021-02622-9</u>; Mostafa A., Scholtes L., Golfier F. (2023), Fuel, 345, 128165, <u>https://doi.org/10.1016/j.fuel.2023.128165</u>