Ph.D. project

Elementary mechanisms of hydro-mechanical deformation in clay and cement: Insight from atomistic and meso-scale modeling

Microporous materials (porous materials with pores smaller than 2nm) are known to exhibit unusual poro-mechanical behaviors, because of the confinement of the fluid in the micropores. Clay- and cement-based materials are some of the most widespread microporous materials, in which confined water is known to induce anomalous hydro-mechanical couplings such as drying shrinkage[1], thermal contraction[2], and accelerated creep rate[3]. A better understanding of those couplings is of prime importance for a variety of applications from the security of geological storage and aging infrastructure to landslide and preservation of cultural heritage. However, the elementary mechanisms of deformation that relates water confinement to the macroscopic response are poorly known, in particular the role of the meso-structure (structure between a few nm and a few μm). Bridging the gap between the molecular and continuum scales could pave the way to strategies for the mitigation or control of hydro-mechanical couplings. The objective of this PhD project is to use molecular and meso-scale modeling to investigate the deformation mechanisms behind hydro-mechanical couplings in clay and cement.

Recent advances in molecular modeling of clay and cement have led to realistic representations of those materials at the nanometer scale, and have provided valuable insight into the physics at the heart of moisture-induced deformations (e.g., disjoining pressure of confined water). In contrast, meso-scale modeling of those materials is still emerging in the scientific community, and little is known about the moisture-induced effects on the meso-structure while experiments point to some major impacts (e.g., pore size distribution).

In this PhD project, we propose to set up a meso-scale model of clay and cement able to coarse-grain the nano-scale behavior provided by molecular simulation. Special attention will be paid to elaborate a realistic coarse-graining of both the compressive and shear interactions between water-covered solid minerals and to account for the mineral flexibility. Existing meso-scale models often focus on the compressive interaction only, but shear and flexibility are potentially critical[4] (e.g., plasticity favored by sliding / limited by elastic energy storage).

A first part of the Ph.D. project will be dedicated to molecular simulations to perform all the characterizations needed for the meso-scale model. This work lies in the continuity of previous studies of the research team[5,6]. A second part of the project will focus on the elaboration of a coarse-grained meso-scale model versatile enough to be adapted to both clay and cement. Likewise, this work will build on recent developments of the research team (cf. illustration). A last part will aim at confronting the outcome of the meso-scale model with available data about hydro-mechanical coupling of clay and cement (e.g., impact of moisture content on pore size distribution, moisture-induced softening).

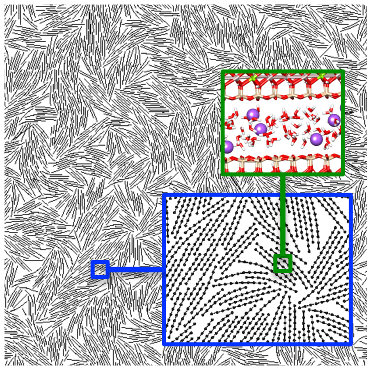

Illustration of the molecular and meso-scale models

The ideal candidate will have a solid background in mechanics and physics of materials with a strong taste for numerical modeling.

Advisors: L. Brochard & M. Vandamme (Laboratoire Navier, Ecole des Ponts ParisTech), T. Honorio & F. Benboudjema (Laboratoire de mécanique et technologie, ENS Paris-Saclay)

Duration: 3 years, starting in Fall 2019

Salary: Net salary of about 1600€ per month

To apply: By 24 March 2019, please send CV, transcripts and motivation letter to laurent.brochard@enpc.fr

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[1] Carrier et al. (2013). Langmuir, 29(41), 12823–12833. http://doi.org/10.1021/la402781p
[2] Brochard et al. (2017). Acta Geotechnica, 12(6), 1261–1279. http://doi.org/10.1007/s11440-017-0596-3
[3] Carrier et al. (2016). Langmuir, 32(5), 1370–1379. http://doi.org/10.1021/acs.langmuir.5b03431
[4] Honorio et al. (2018). Soft Matter, 14(36), 7354–7367. http://doi.org/10.1039/C8SM01359D
[5] Honorio et al. (2017). Langmuir, 33(44), 12766–12776. http://doi.org/10.1021/acs.langmuir.7b03198
[6] Honorio (2019). Langmuir, accepted. http://doi.org/10.1021/acs.langmuir.8b04156