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Hydromechanical couplings in the clay matrix of argillite: some methodological aspects of the atomistic-to-continuum upscaling

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Abstract :

Clays are ubiquitous in civil engineering applications, from deep geological disposal of radioactive waste to petroleum engineering, all of which require a good knowledge of their mechanical properties. Swelling clays are highly sensitive to the relative humidity: increases of water content can induce significant volume increases, as well as variations of the elastic stiffness. A faithful description of the behavior of clayey materials must therefore account for the hydromechanical couplings within clays.

Hydromechanical couplings within the clay matrix of argillite were investigated numerically following a multi-scale approach. At the smallest scale, the clay layers of Na-montmorillonite are characterized through Monte Carlo molecular simulations. The constitutive law of the particle (a stack of clay layers) is then derived through rheological models. Finally, the clay matrix is represented as a polycrystal made of clay particles and homogenized by means of numerical non-linear continuum mechanics methods.

Throughout our investigations, it was realized that the atomistic-to-continuum scale transition raised non-trivial theoretical questions. In this poster, we propose to show how the output of molecular simulations can be rigorously fed into a continuum mechanics simulation. Although the issues raised in this poster are illustrated on the upscaling of Na-montmorillonite, they are of a methodological nature and have a much wider range of applications.

Keywords : molecular simulations; numerical homogenization; finite strains

According to [1], the clay layer can be seen as a microporous medium. Deformation and addition/removal of water molecules to this system results in a change of the Helmholtz free energy per unit undeformed volume, f , according to the following energy balance

$$df = \mathbf{S} : d\mathbf{E} + \mu dn,$$

where \mathbf{S} and \mathbf{E} are work-conjugate stress and strain measures, n is the inter-layer water content (in moles of water per unit undeformed volume) and μ is the molar chemical potential of water. In other words, the behavior of the clay layer is characterized through two state variables, one of which must belong to the set $\{\mathbf{S}, \mathbf{E}\}$, the other to the set $\{n, \mu\}$.

In [2, 3], Monte Carlo molecular simulations were carried out in the grand canonical and isobaric ensemble. From isobaric simulations (where the state variables are \mathbf{S} and n) were derived the swelling curves (interlayer distance as a function of the water content at fixed stress) as well as the tangent stiffness. Water adsorption isotherms (water content as a function of the chemical potential at fixed strain) were then computed in the grand canonical ensemble (where the state variables are \mathbf{E} and μ). In order to be able to feed unambiguously this data into a continuum mechanics simulation, several questions had to be answered.

First, the exact nature of the tangent stiffness computed through MC simulations had to be clarified. Tangent stiffnesses relate stress-increments to strain-increments. Since changes in water content may

induce very large strains (up to 100 %) in clay layers, it is crucial (in a finite strain framework) to understand the exact nature of stress and strain measures implicitly used in molecular simulations. We will show how we made sure that the tangent stiffness returned by our simulations related the work-conjugate Piola II stress \mathbf{S} to the Green-Lagrange strain \mathbf{E} .

Second, the formulation of a constitutive law requires the definition of a reference configuration. The natural choice is of course the stress-free configuration. However, such configuration is not unique for swelling clays (it depends on the water content n). Therefore, an arbitrary reference configuration had to be chosen, and we will show how the output of the molecular simulations had to be corrected to account for this choice.

Third, the natural state variables for the continuum mechanics simulations are the strain \mathbf{E} and the chemical potential μ (since the ambient relative humidity is usually controlled). In the language of standard poromechanics, *drained* elastic moduli are required. However, the elastic moduli derived from molecular simulations were obtained at fixed water content, which correspond to *undrained* elastic moduli in standard poromechanics. We will show how the undrained stiffness and water adsorption isotherms can be combined to derive the drained stiffness.

All these points will be illustrated in the case of Na-montmorillonite, where it will be shown numerically that failing to account for any of these issues can lead to significant errors.

To conclude this poster, we will outline the remaining work of this project, namely the determination of scale transitions to the clay particles first, then to the clay matrix. Clay particles are regarded as stacks of clay layers, and simple rheological models are used to compute their effective behavior. This model must account for the co-existence of several hydration states at given relative humidity: these states have been identified through our molecular simulations, which will be complemented with experimental data [4]. The clay matrix is represented as a polycrystal, where the orientations of the monocrystals are distributed according to experimental XRD data [5]. A voxel-based, non-linear continuum mechanics technique [6] is then used to homogenize the resulting microstructure.

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