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

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Context

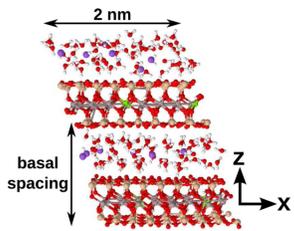
- > Clays are ubiquitous in civil engineering applications
- > Good knowledge of their mechanical behaviour is necessary
- > Swelling clays are highly sensitive to relative humidity
- > Hydromechanical couplings *must* be accounted for

$$\sigma = f(\varepsilon, RH)$$

Aim of this study

- > Modelling of hydromechanical couplings in the clay matrix of argilite
- > Investigation of the influence of local orientational order

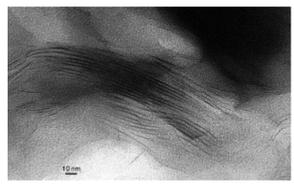
Numerical, multi-scale approach



Microscopic scale : the clay sheet

- > Molecular dynamics (μ VT and N Σ T)
- > Models developed by Carrier
- > Uses theoretical model of Brochard et al. (2012)

Brochard (2012), JMPs 60(4), 606
Carrier (2013), PhD Thesis, Université Paris-Est
Carrier et al. (2014), J. Phys. C 118(17), 8933



Mesoscopic scale : the clay particle

- > Rheological models
- > Particle viewed as a stack of sheets



Macroscopic scale : the clay matrix

- > Viewed as a polycrystal
- > FFT-based homogenization methods

Brisard and Dormieux (2010), Comp. Mat. Sci. 49(3), 663
Brisard and Dormieux (2012), CMAME 217-220, 197

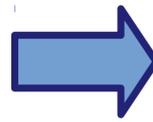
Finite strains formulation of molecular simulations

- > How to make sure that molecular simulations return the "right" stiffness?
- > Need to understand how N Σ T simulations are run
- > Change of geometry of the unit-cell is accepted with probability

$$p \propto \exp\left(-\frac{S(E_{\text{new}} - E_{\text{old}})}{kT}\right)$$

E_{old} strain in the old configuration (measured)
 E_{new} strain in the new configuration (measured)
 S stress (imposed)

This is an energy change!



- > Like in mechanics, S is dual to E .
- > The nature of S depends on how we measure E .
- > If we measure a GL strain, then S is the Piola II stress.

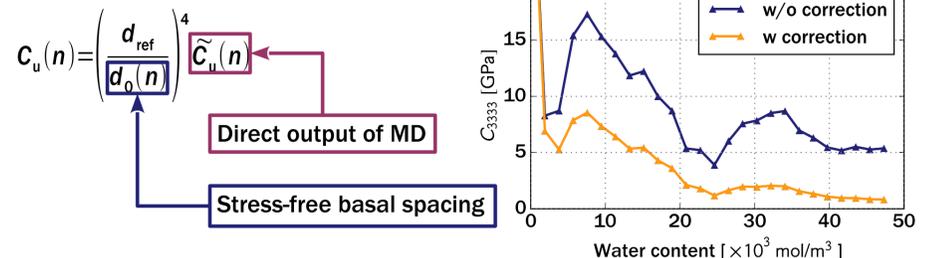
On the reference configuration

- > Strains are measured with respect to a reference configuration
- > The stress-free configuration is not unique (depends on the water content)
- > Prestressed reference configuration

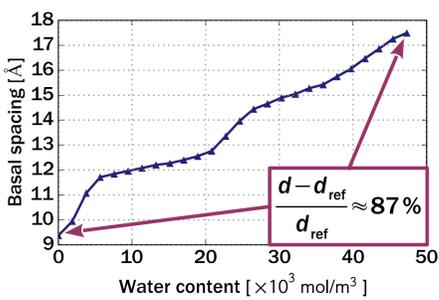
$$S = C_u(n) E - E_0(n)$$

Free hydric strain
Undrained stiffness

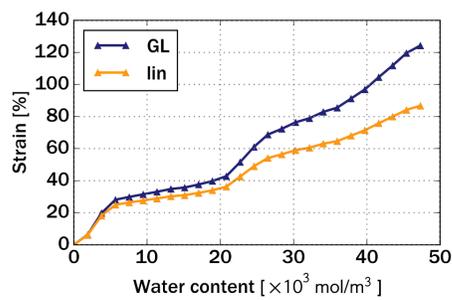
- > Correction of molecular dynamics results



Finite strains induced by changes in RH

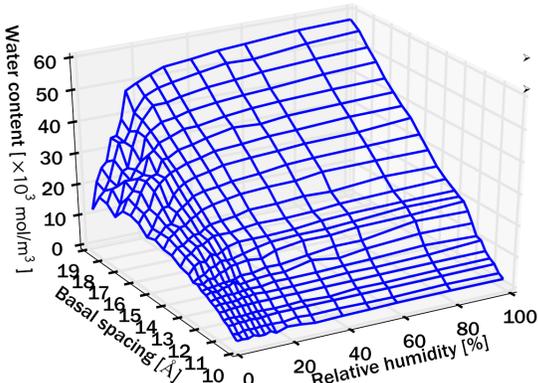


Green-Lagrange strain



$$E = \frac{d - d_{\text{ref}}}{d_{\text{ref}}} + \frac{1}{2} \left(\frac{d - d_{\text{ref}}}{d_{\text{ref}}} \right)^2$$

Adsorption isotherms (from B. Carrier, op. cit.)



- > Extensive dataset is available
- > Derivation w.r.t. RH , d not trivial due to statistical errors: work in progress!

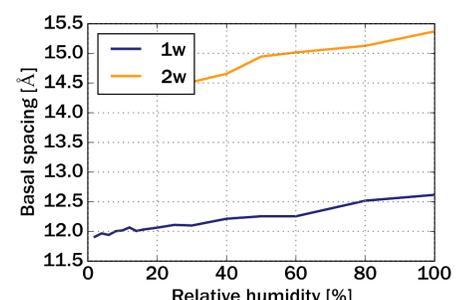
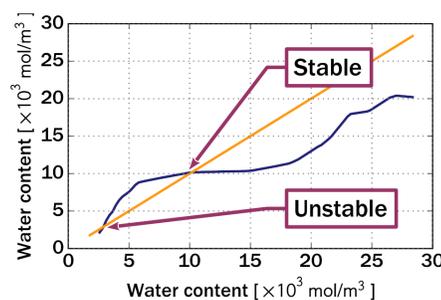
Undrained vs. drained stiffness

- > In our MD simulations, the water content is fixed: undrained stiffness $C_u(n)$
- > In the continuum mechanics simulations (at the scale of the clay matrix), we control the relative humidity (or chemical potential of water): drained stiffness $C_d(\mu)$
- > We need to perform a change of state variables $(E, n) \rightarrow (E, \mu)$

$$C_d(\mu) = C_u(n) - \left(\frac{\partial n}{\partial \mu}\right)^{-1} \left(\frac{\partial n}{\partial E}\right)^2$$

- > Requires the adsorption isotherm $n(d, \mu)$ and its derivatives!

Application: stable equilibria at fixed relative humidity



$$\text{Fixed-point equation } n_{\text{mc}}(d_0(n), \mu) = n$$

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