Using numerical homogenization to compute the mechanical response of Gas Hydrate Bearing Sediments

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Introduction

Gas hydrates are crystalline solids made up of natural gas (typically methane) and water molecules. They form under high pressure and low temperature conditions, which is naturally possible along the continental margins. Because they represent both a potential energy resource and a threat to the stability of the seafloor, it is important to be able to predict the mechanical behaviour of gas hydrate bearing sediments.

Two-scale finite-element model

The mechanical behaviour of a REV of sediments, regarded as a homogeneous material, can be modeled with a finite-element code, in which each element stiffness matrix has to be evaluated with numerical integrations. To perform these integrations the Gaussian integration scheme is commonly used and it needs to calculate the constitutive matrix $[C]$ at each integration point:

$$d\sigma = [C]d\varepsilon.$$

Due to the complex microstructure and instability of gas hydrate bearing sediments, no recognized constitutive behavior exists so the choice of a constitutive matrix remains uncertain. The models published in the literature are usually based on classic elasto-plastic models such as the Modified Cam-Clay model (Kimoto et al., 2010;Uchida et al., 2012) or the elastic-perfectly plastic model with the Mohr-Coulomb yield criterion (Klar et al., 2010). The authors enhanced these models by introducing new parameters taking the effect of the hydrate volume fraction in the soil into account, the parameters being calibrated to fit experimental results.

To overcome the complex determination of such parameters, one possible way is to calculate $[C]$ through a homogenization technique based on Fast Fourier Transforms (FFT). A heterogeneous microscopic unit-cell containing the different phases of the material (hydrate inclusions, sand grains, clay, voids) is assigned to each Gauss point. This two-scale finite-element-FFT model is employed to numerically assess the impact of the microstructure, like the morphology of the sediments and gas hydrates.

Numerical homogenization using FFT-based methods

Homogenization methods provide the macroscopic behaviour of a heterogeneous Representative Elementary Volume (REV). They can help model the mechanical behaviour of gas hydrate bearing sediments in the absence of reliable experimental properties. Indeed, characterizing the mechanical response of these sediments under *in situ* conditions is still a challenging process (Hyodo et al., 2013;Yoneda et al., 2015). Fast Fourier Transforms represent an easy way to solve the local mechanical problem of an elementary composite cell, under periodic boundary conditions for fluctuating displacements and anti-periodic boundary conditions for tractions (Moulinec and Suquet, 1998). These frequency based methods have a low computational cost since they do not need any mesh and are suitable for parallel computing. They also enable each constituent of the composite to have either a linear or nonlinear constitutive behaviour (Moulinec and Suquet, 1998;Gélébart and Mondon-Cancel, 2013).

In the FFT-based homogenization methods, a unit-cell representing the microstructure of a composite is discretized into a regular grid of 'pixels' (2D) or 'voxels' (3D), and defined by a pixel-wise (or voxel-wise) constant local constitutive equation. This unit-cell is also submitted to a macroscopic load, which can be a uniform strain or a uniform stress. We only focus on cases with prescribed macroscopic strain E, because it corresponds to the finite-element numerical integration scheme in the perspective of multi-scale approaches. The strain and displacement fields are then separated as follows, x being the coordinates of pixels in real space:

$$\begin{cases} \varepsilon\big(u(x)\big) = \varepsilon\big(u^*(x)\big) + E \\ u(x) = u^*(x) + E.x \end{cases},$$

with local fluctuating terms $\varepsilon(u^*(x))$ and $u^*(x)$ the average of which is null. The introduction of a homogeneous 'reference material' with an elastic stiffness tensor C^0 and a polarization field $\tau(x)$ leads to the Lippmann-Schwinger (L.-S.) equation as the new equation of the local problem (Moulinec and Suquet, 1994):

$$\begin{cases} \varepsilon\big(u(x)\big) = -\Gamma^0(x) * \tau(x) + E \quad \forall x \qquad (Real\ space) \\ \quad \hat{\varepsilon}(\xi) = -\hat{\Gamma}^0(\xi) : \hat{\tau}(\xi) \quad \forall \xi \neq 0, \quad \hat{\varepsilon}(0) = E \qquad (Fourier\ space) \end{cases},$$
$$\tau(x) = \sigma(x) - C^0 : \varepsilon\big(u(x)\big),$$

where $(*)$ is the convolution product, ξ is the frequency in Fourier space, and Γ^0 the Green operator associated with C^0. Frequencies are also discretized corresponding to the real space discretization of the unit-cell. The solution strain and stress fields are obtained by solving the L.-S. implicit equation. This equation is more conveniently computed in Fourier space where the convolution product is avoided, hence the need to use Fast Fourier Transforms. Different algorithms can be used to solve the equation, the 'Basic Scheme' (Moulinec and Suquet, 1994) is based on the fixed point algorithm for example. The macroscopic stress response is evaluated by averaging the local stress field over the unit-cell. When one or more of the phases of the composite has a nonlinear constitutive law, the loading path $[0; E]$ is discretized into subintervals $[E_{n-1}; E_n]$ and at each step n the L.-S. equation becomes:

$$\hat{\varepsilon}_n(\xi) = -\hat{\Gamma}^0(\xi) : \big(\hat{\sigma}_n(\xi) - C^0 : \hat{\varepsilon}_n(\xi)\big) \quad \forall \xi \neq 0, \quad \hat{\varepsilon}_n(0) = E_n \qquad (Fourier\ space),$$

with (σ_n, p_n) being computed from $(\varepsilon_n, \sigma_{n-1}, \varepsilon_{n-1}, p_{n-1})$, and p representing internal variables.

Knowing the local constitutive behaviour (linear elasticity, nonlinear elasticity, elasto-plasticity,...) of each constituent of a REV of gas hydrate bearing sediments, one can finally compute its response to a uniform strain load (see Fig.1).

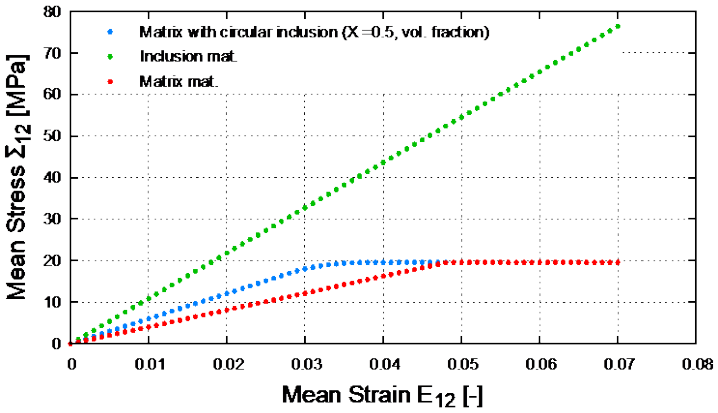

Fig.1: Stress-strain curve resulting from a FFT-based homogenization (in blue) of a unit-cell comprising an elastic-perfectly plastic soil matrix (red) and an elastic inclusion (green) of 0.5 volume fraction

Conclusion

The application of multi-scale approaches in the establishment of a numerical model for gas hydrate bearing sediments is an interesting way to overcome the difficulties of experimental researches. The mechanical behaviour of the REV is obtained through a computational efficient homogenization calculation based on FFT.

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