

A MULTI-SCALE COMPUTATIONAL SCHEME FOR ANISOTROPIC HYDRO-MECHANICAL COUPLINGS IN SATURATED HETEROGENEOUS POROUS MEDIA

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Abstract. This contribution discusses a coupled two-scale framework for hydro-mechanical problems in saturated heterogeneous porous geomaterials. The heterogeneous nature of such materials can lead to an anisotropy of the hydro-mechanical couplings and non-linear effects. Based on an assumed model of the mesostructure, the average macroscopic hydro-mechanical behaviour is extracted by means of a computational homogenisation procedure in a monolithic way. The ingredients needed to upscale the hydro-mechanical couplings are outlined. The two-scale simulation results are compared with direct numerical simulation for the consolidation of a particle-matrix porous material.

1 INTRODUCTION

The formulation of macroscopic constitutive laws for the hydro-mechanical behaviour of heterogeneous porous geomaterials such as masonry, concrete or soil is complex. Due to the hydro-mechanical couplings, non-linear effects such as stress-induced permeability evolution may occur. The mesostructure of geomaterials may also result in the appearance of anisotropic hydro-mechanical properties. The characterisation of such a behaviour by means of macroscopic closed-form constitutive laws is difficult because of their complex formulation and the costly identification of their parameters. As a complementary approach, multi-scale computational strategies aim at solving this issue by deducing a homogenised response at struc-

tural scale from a representative volume element of the fine scale (RVE), based on constituents properties and averaging theorems, see Figure 1. The constituents inside the RVE may be modelled using a closed-form formulation, depending on the multi-physical phenomena to be represented. A variational homogenisation procedure taking into account fine-scale transient phenomena and based on (strong) uniform boundary conditions applied to the fine-scale RVE was recently proposed for consolidation problems in [1]. Here, a formulation using periodic computational homogenisation will be proposed for saturated heterogeneous porous media. The fine-scale constituents considered here are made of a heterogeneous porous solid skeleton saturated with a compressible pore fluid

such as water and are themselves represented as homogeneous media. The heterogeneities in the mechanical, hydraulic and coupling properties of the solid phases are thus considered at the RVE level.

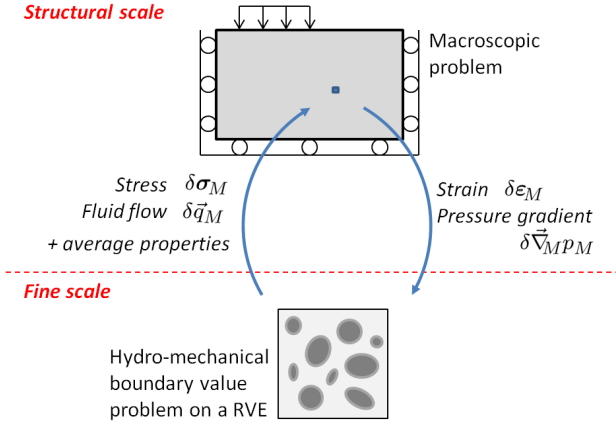


Figure 1: Principle of a two-scale nested computational procedure for saturated hydro-mechanical problems.

2 COMPUTATIONAL HOMOGENISATION

Computational homogenisation approaches allow identifying equivalent homogenised continuum properties from the constituents constitutive behaviour of a heterogeneous mesostructural RVE. The behaviour of each constituent within the mesostructural RVE is assumed to be a priori known. This allows the set-up of nested computational procedures in which a sample of the mesostructure is used to numerically determine the local macroscopic material response of the heterogeneous material. The definition of such a nested scheme essentially requires the definition of four ingredients: (i) a fine-scale constitutive description for the constituents, (ii) the definition of a representative mesostructural sample, (iii) the choice of a coarse-scale representation, and (iv) the set-up of scale transitions linking structural and fine-scale quantities.

Such methods were developed for the mechanical case in [2] and for thermo-mechanical problems in [3, 4] using a staggered approach. Based on these methods, the scale-transitions are here adapted for saturated hydro-mechanical problems in a monolithic way based

on fine-scale steady-state information and periodicity constraints applied at the boundary of the RVE. Such constraints are classically related to the assumption of the separation of scales; the material configuration is macroscopically homogeneous, but mesoscopically heterogeneous [2].

3 TWO-SCALE FRAMEWORK FOR SATURATED POROUS MEDIA

3.1 Macroscopic description

At the macroscopic scale, a classical porous medium assumption [5] including material nonlinearities is used to model the (evolving) equivalent hydro-mechanical properties under quasi-static conditions in the infinitesimal range of deformation. The balance equations consist of the momentum equilibrium and the mass conservation equation

$$\vec{\nabla}_M \cdot \boldsymbol{\sigma}_M + \vec{b} = \vec{0} \quad (1)$$

$$\dot{\zeta}_M + \vec{\nabla}_M \cdot \vec{q}_M = Q_s \quad (2)$$

where $\boldsymbol{\sigma}_M$ is the total stress tensor, \vec{b} is the body force vector, ζ_M is the fluid content increment, \vec{q}_M is the fluid flow vector and Q_s is a body flow source. $\vec{\nabla}_M$ is the gradient operator with respect to the coordinates at the macroscopic scale. The total stress state of a fluid-saturated porous medium is usually decomposed into an effective stress state $\boldsymbol{\sigma}_M^{\text{eff}}$ of the solid skeleton and a fluid pressure p_M as follows

$$\boldsymbol{\sigma}_M = \boldsymbol{\sigma}_M^{\text{eff}} - \boldsymbol{\alpha}_M p_M \quad (3)$$

where $\boldsymbol{\alpha}_M$ is the second-order Biot coefficient tensor associated with the hydro-mechanical couplings. The multi-physical couplings of geomaterials generally present an initial anisotropy [6] which can evolve due to damage [7]. The quasi-brittle mechanical behaviour of geomaterials is usually driven by a non-linear constitutive law linking in a variational form the variation of the effective stress tensor to variation of the strain tensor $\boldsymbol{\varepsilon}_M = (\vec{\nabla}_M \vec{u}_M)^{\text{sym}}$ of the solid skeleton

$$\delta \boldsymbol{\sigma}_M^{\text{eff}} = {}^4\mathbf{C}_M : \delta \boldsymbol{\varepsilon}_M \quad (4)$$

where ${}^4\mathbf{C}_M$ is the tangent stiffness tensor of the solid phase. The fluid transport within the porous medium is driven by Darcy's law

$$\vec{q}_M = -\kappa_M \vec{\nabla}_M p_M \quad (5)$$

where κ_M is the permeability tensor. This parameter can evolve, for instance, in terms of the effective stress state in geomaterials susceptible to damage [8]. The increment of the fluid content is a storage function which depends on both the mechanical and hydraulic behaviour as follows

$$\zeta_M = \alpha_M : \varepsilon_M + \frac{1}{M} p_M \quad (6)$$

where $1/M$ is the compressibility modulus. This parameter will be assumed constant for the sake of simplicity.

3.2 Fine-scale description

In the context of a multi-scale framework, the equivalent macroscopic (hydro-mechanical) behaviour is obtained by means of nested computations performed on a RVE where the heterogeneities observed at the fine scale are modelled. This framework is called FE² if finite element modelling is used at both scales. At the fine scale, any mesostructure and closed-form law can be a priori postulated. In order to focus on the upscaling of the coupled hydro-mechanical properties, a mesostructure consisting of a matrix with a single poroelastic inclusion will be considered.

At fine scale, since the RVE size is assumed to be small with respect to the structural dimensions (separation of scales), the fine-scale transient effects are neglected, assuming a steady-state (instantaneous) hydro-mechanical equilibrium within the RVE, in the same spirit as [3]. Neglecting body forces and sources inside the RVE, the fine-scale hydro-mechanical balance equations therefore read

$$\vec{\nabla}_m \cdot \boldsymbol{\sigma}_m = \vec{0} \quad (7)$$

$$\vec{\nabla}_m \cdot \vec{q}_m = 0 \quad (8)$$

where $\boldsymbol{\sigma}_m$ is the fine-scale total stress tensor and \vec{q}_m is the fine-scale fluid flow vector. $\vec{\nabla}_m$

is the gradient operator with respect to the coordinates at RVE level. Note that due to the steady-state assumption, both the hydraulic and mechanical problems have the same format, i.e. divergence-free balance equations. Note also that the fluid content increment and the compressibility modulus are not taken into account at this level. Only the tangent stiffness ${}^4\mathbf{C}_M$, the permeability κ_M and the hydro-mechanical coupling α_M take part in the formulation. In this contribution, elastic properties with a stress dependent permeability and anisotropic hydro-mechanical couplings will be considered.

3.3 Non-linear homogenisation of coupled hydro-mechanical properties

The equivalent macroscopic hydro-mechanical properties of a heterogeneous porous mesostructure can be deduced from a steady-state hydro-mechanical problem solved on a RVE. The link between the macroscopic and fine scales is ensured by means of averaging relations. For the mechanical case, the consistency between scales is enforced for the strain, the stress and the work variables, see [2]. For the hydraulic case, averaging relations are defined for the pressure gradient, the flow and the entropy variables, by analogy with the thermal case developed in [3]. All these averaging relations can be satisfied by appropriate boundary conditions at the boundary of the RVE, among which the periodicity constraints are the most used.

Based on the macroscopic strain and pressure gradient, the fine-scale displacement and pressure profiles within the RVE can be expressed respectively by

$$\vec{u}_m(\vec{x}) = \boldsymbol{\varepsilon}_M \cdot \vec{x} + \vec{u}_f(\vec{x}) \quad (9)$$

$$p_m(\vec{x}) = p_m^k + \vec{\nabla}_M p_M \cdot (\vec{x} - \vec{x}^k) + p_f(\vec{x}) \quad (10)$$

$$(11)$$

where p_m^k is the pressure at an arbitrary point \vec{x}^k . $\vec{u}_f(\vec{x})$ and $p_f(\vec{x})$ are the displacement and pressure fluctuation fields, respectively. These fluctuations are assumed periodic, i.e. taking equal values on any two boundary points on the edges

related by the periodicity relation [2, 3]. Such fluctuations allow accounting for the material heterogeneity inside the RVE for the hydraulic and mechanical behaviours as well as their couplings.

On the basis of the periodicity assumption, the averaging relations allow one formulating a boundary value problem on the RVE and controlling its behaviour from degrees of freedom at specific controlling points [2, 3]. The strain measure ϵ_M and the pressure gradient measure $\vec{\nabla}_M p_M$ of the macroscopic description can then be expressed in terms of controlling degrees of freedom of the discretised RVE (three controlling dofs for the strain and two controlling dofs for the pressure gradient).

The rigid body translations of the RVE are implicitly inhibited by means of the assumed displacement profile (9) without loss of generality. For the hydraulic case, since the (usual) averaging relation is assumed for the gradient of the pressure field, the fluid pressure level at the fine scale can not be determined in a unique way with this relation only. This level however has to be prescribed properly inside the RVE since it directly contributes to the total stress level due to the hydro-mechanical coupling (3). Note that the macroscopic pressure p_M cannot be directly applied on a fine-scale node. By analogy with [3], this motivates to impose an additional consistency (averaging relation) for the pressure field between the macroscopic and fine scales which reads

$$p_M = \frac{1}{V} \int_V p_m dV \quad (12)$$

where V is the RVE volume. Using a finite element discretisation, Equation (12) leads to a non-homogeneous tying relation. A phantom node method can be used to prescribe the independent term of this relation. A controlling degree of freedom associated to this term is therefore added to the fine-scale system in order to impose in an average sense the macroscopic pressure level p_M . Note that this tying relation involves all the degrees of freedom of pressure which significantly increases the band width of

the system to solve. The macroscopic pressure gradient is also imposed in an average sense by using non-homogeneous tying constraints.

Using the periodic displacement and pressure boundary conditions, and the pressure consistency between scales (12), the fine-scale steady-state hydro-mechanical problem can be solved in a monolithic way. The average macroscopic response, i.e. the total stress and the fluid flow, can be extracted from the response of the RVE condensed at the controlling degrees of freedom. The macroscopic tangent stiffness, permeability and the hydro-mechanical coupling coefficients can also be extracted from the condensation of the fine-scale system matrix. Note that the upscaling of the coupling coefficients is allowed by the additional degree of freedom controlling the macroscopic pressure level within the RVE and introduced by the pressure consistency between scales (12).

Since transient phenomena are neglected at fine scale, the fluid content increment and the compressibility modulus can not be deduced from the RVE response condensed at the controlling degrees of freedom. The macroscopic compressibility modulus is therefore deduced from fine-scale quantities by an explicit volume integral on the RVE. The macroscopic fluid content increment is then deduced by Equation (6).

4 COMPARISON OF MULTI-SCALE AND FINE-SCALE RESULTS ON TEXTURED POROUS MATERIALS

The proposed multi-scale scheme was implemented using parallel computation. Two cases of consolidation of heterogeneous textured porous materials are considered to illustrate the non-linear homogenisation procedure. A periodic poroelastic inclusion-matrix material is considered. A non-linearity is introduced in the fluid transport by making the permeability dependent of the effective stresses, and the anisotropy of the hydro-mechanical coupling is studied. The multi-scale solutions (MS) are compared to direct numerical simulations (DNS) used as a reference, keeping in mind that

the scale separation assumption of the computational homogenisation procedure is not exactly satisfied here.

4.1 Stress-induced permeability evolution

The considered consolidation case is a confined column of dimensions $0.2 \times 1 \text{ m}^2$ with a uniformly distributed compressive load of 1 MPa instantaneously applied on the top surface. The top surface is permeable at a constant pressure prescribed to zero and the other edges are impervious to fluid flow. The fine-scale structure is a periodic arrangement of square inclusions embedded in a more permeable and softer matrix. The unit cell used for the multi-scale computation is therefore a square with a centered square particle, see Figure 2. The dimensions of the unit cell are $0.05 \times 0.05 \text{ m}^2$ and the inclusion volume is around 50% of the cell volume. The material properties are heterogeneous with respect to the elastic behaviour and the permeability, see Table 1. An arbitrary closed-form law is chosen for the permeability in terms of the effective stress in order to introduce non-linearity in the problem. The permeability of the matrix linearly depends on the volumetric effective stress as follows [7]

$$\kappa = \kappa_i(1 + A\sigma_v^{\text{eff}}) \quad (13)$$

where A is a constant coefficient, leading to a decrease of permeability with volumetric compression. The permeability of the inclusion is kept constant, see Table 1. This case is compared to the case where the permeability of the matrix is independent of the stress state ($\kappa = \kappa_i$ or $A = 0$).

Table 1: Matrix (a) and inclusion (b) material parameters. E is the Young modulus and ν is the Poisson ratio.

| | (a) | (b) |
|--|--------------------|---------------------|
| E (GPa) | 1 | 10 |
| ν (-) | 0.4 | 0.1 |
| M (GPa) | 5 | 5 |
| α (-) | 0.5 | 0.5 |
| κ_i ($\text{m}^2/\text{Pa}\cdot\text{s}$) | 3×10^{-9} | 3×10^{-10} |
| A (MPa^{-1}) | 1 | 0 |

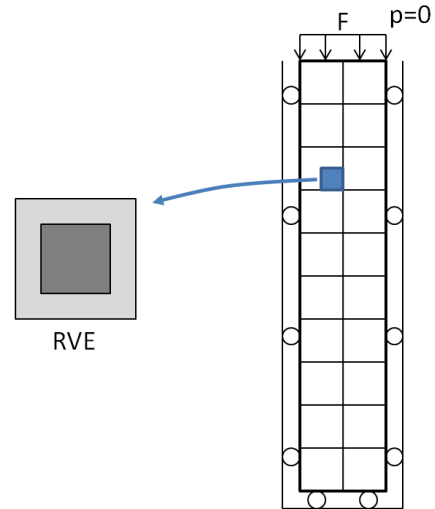


Figure 2: Configuration of the consolidation of a heterogeneous porous material made of a periodic arrangement of square inclusions.

The time evolution of the pressure at the bottom of the column is depicted in Figure 3 for both constant and evolving permeability and for both fine-scale and multi-scale models. The settlement evolution is also shown in Figure 4. Note that the settlement is taken at the mid-depth of the column to avoid top boundary effect. The heterogeneities of both the mechanical and hydraulic properties are correctly taken into account by the multi-scale model. The decrease of the permeability and the related slower decrease of the pressure with consolidation is also well captured by the homogenisation procedure.

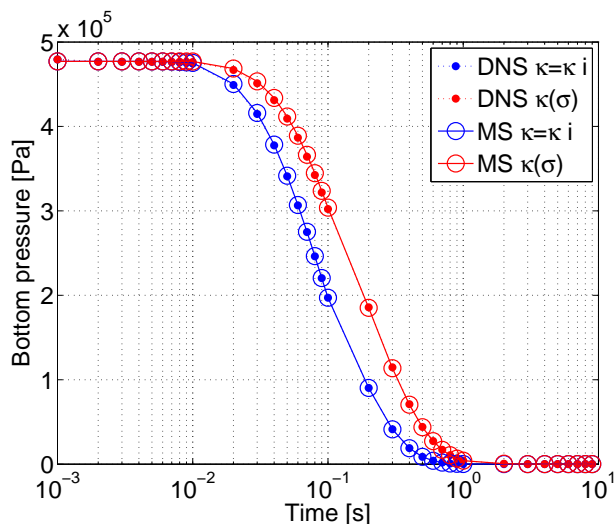


Figure 3: Consolidation of a heterogeneous porous material with constant permeability (blue) and evolving permeability (red). Comparison of the bottom pressure evolution for direct numerical simulation (DNS - dot markers) and multi-scale simulation (MS - circle markers).

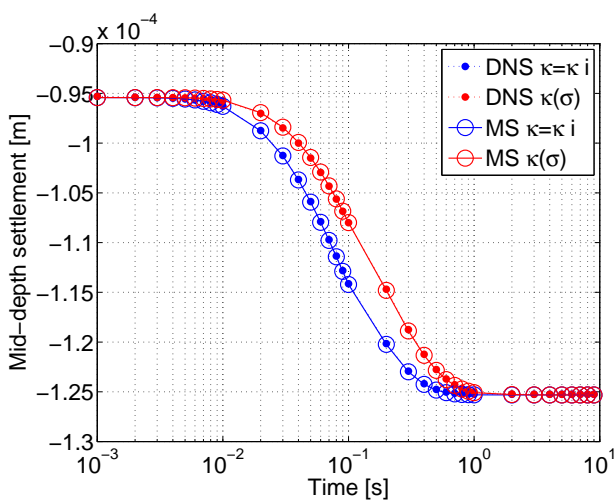


Figure 4: Consolidation of a heterogeneous porous material with constant permeability (blue) and evolving permeability (red). Comparison of the mid-depth settlement evolution for direct numerical simulation (DNS - dot markers) and multi-scale simulation (MS - circle markers).

4.2 Anisotropic hydro-mechanical couplings

In order to introduce anisotropy, the same case of consolidation is revisited with vertical and horizontal rectangular inclusions, as depicted in Figure 5. The ratio of inclusion-matrix

volume is preserved with respect to the case of square inclusions used in the previous example. Heterogeneous elastic properties are considered with identical permeability in both matrix and inclusion materials in order to focus on the effect of an anisotropic hydro-mechanical coupling. Homogeneous and heterogeneous Biot coefficients are successively considered for both fine-scale structures (vertical and horizontal inclusion), see Table 2. Each multi-scale solution is compared to the results of a direct numerical simulation.

Table 2: Matrix (a) and inclusion (b) material parameters for the homogeneous (hmg) and heterogeneous (htg) cases regarding the Biot coefficient.

| | hmg | | htg | |
|--|---------------------|-----|---------------------|-----|
| | (a) | (b) | (a) | (b) |
| E (GPa) | 1 | 10 | 1 | 10 |
| ν (-) | 0.4 | 0.1 | 0.4 | 0.1 |
| M (GPa) | 5 | 5 | 5 | 5 |
| α (-) | 0.5 | 0.5 | 0.5 | 1 |
| κ ($\text{m}^2/\text{Pa}\cdot\text{s}$) | 3×10^{-13} | | 3×10^{-13} | |

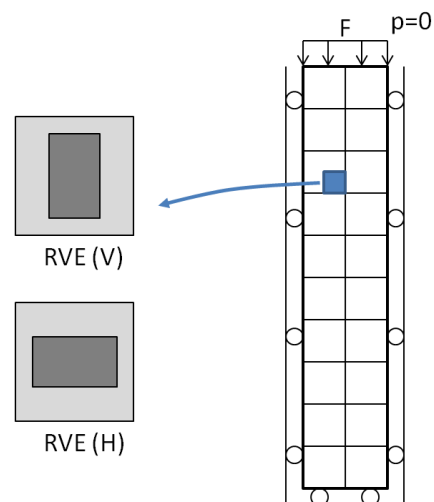


Figure 5: Configurations of the consolidation of a heterogeneous porous material made of a periodic arrangement of either vertical (V) or horizontal (H) rectangular inclusions.

The bottom pressure evolution and the mid-depth settlement are presented in Figures 6 and 7, respectively. Since the pressure vanishes at

the end of each simulation, only the first time steps are shown. It is observed that the heterogeneity of the hydro-mechanical coupling (in blue) is properly captured by the homogenisation procedure with respect to the cases where a homogeneous coupling is used (in red). At the first time step, the multi-scale solution overestimates the pressure with an error of less than 5% and underestimates the displacement with an error of 2.2% (with respect to the DNS). This error is decreasing with time and only the anisotropy of the elastic parameters affects the steady-state (final) settlement. The periodicity condition imposed on the displacement and pressure fields and the fact that the scale separation is not satisfied here could explain the initial overestimation of the undrained stiffness. The steady-state assumption at the fine scale could also be an origin of the discrepancy between the multi-scale and fine-scale results since the fluid content increment depends on the Biot coefficients.

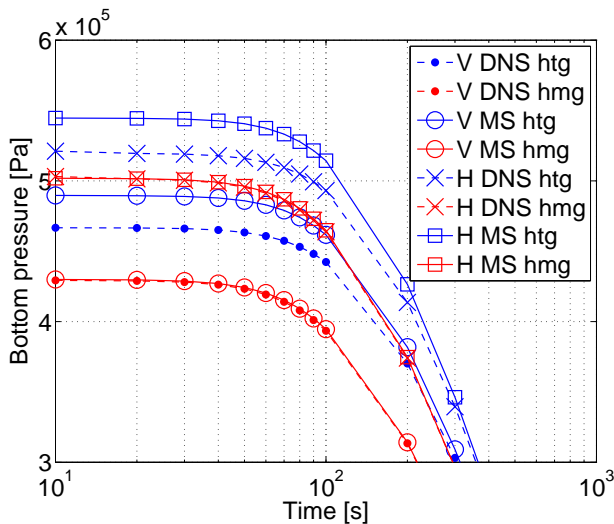


Figure 6: Consolidation of a heterogeneous porous material with vertical (V) and horizontal (H) inclusions for homogeneous (hmg - red) and heterogeneous (htg - blue) Biot coefficients. Comparison of the mid-depth settlement evolution for direct numerical simulation (DNS - dot and cross markers) and multi-scale simulation (MS - circle and square markers).

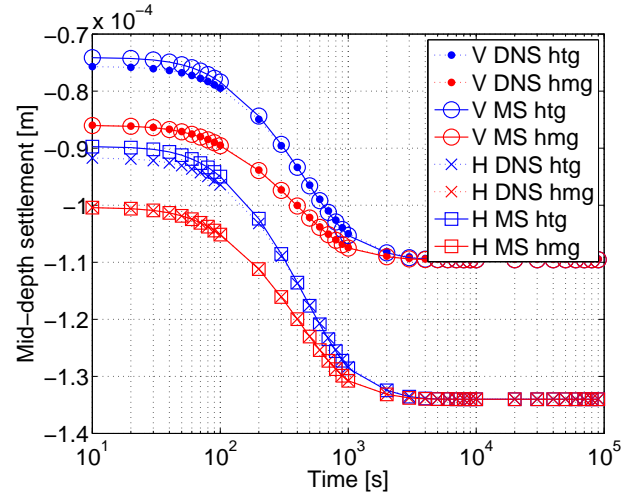


Figure 7: Consolidation of a heterogeneous porous material with vertical (V) and horizontal (H) inclusions for homogeneous (hmg - red) and heterogeneous (htg - blue) Biot coefficients. Comparison of the mid-depth settlement evolution for direct numerical simulation (DNS - dot and cross markers) and multi-scale simulation (MS - circle and square markers).

5 CONCLUSIONS

A non-linear computational homogenisation procedure was proposed for the hydro-mechanical behaviour of saturated heterogeneous porous materials. Based on computational homogenisation approaches developed for the mechanical and thermal cases [2, 3], an enhancement of the scale transitions by means of a consistency between scales on the pressure field is proposed. It allows accounting for the hydro-mechanical couplings in a monolithic way. It was shown that the multi-scale modelling yields results in good agreement with respect to direct numerical simulations results for consolidation cases in terms of displacement and pressure evolution. In particular, the multi-scale methodology allows taking into account a stress-induced permeability evolution and an anisotropy of the hydro-mechanical couplings. The periodicity argument and the influence of the fine-scale transient phenomena should be addressed in forthcoming publications. As a perspective, the methodology proposed in [9, 10] where RVE computations are used to model localised mechanical behaviour will be extended for the case of hydro-

mechanical couplings. A damage model including hydro-mechanical couplings will be incorporated at the RVE level in order to capture damage-induced anisotropy with cracking and fluid flow inside cracks.

REFERENCES

- [1] Su, F., Larsson, F. and Runesson, K., 2011. Computational homogenization of coupled consolidation problems in micro-heterogeneous porous media. *Int. J. Num. Meth. Engng.* **88**:1119–1218.
- [2] Kouznetsova, V.G., Brekelmans, W.A.M. and Baaijens, F.P.T., 2001. An approach to micro-macro modeling of heterogeneous materials. *Comput. Mech.* **27**:37–48.
- [3] Ozdemir, I., Brekelmans, W.A.M. and Geers, M.G.D., 2008. Computational homogenization for heat conduction in heterogeneous solids. *Int. J. Num. Meth. Engng.* **73**:185–204.
- [4] Ozdemir, I., Brekelmans, W.A.M. and Geers, M.G.D., 2008. FE² computational homogenization for the thermo-mechanical analysis of heterogeneous solids. *Comput. Methods Appl. Mech. Engrg.* **198**:602–613
- [5] Biot, M.A., 1941. General theory of three-dimensional consolidation. *J. Appl. Phys.* **12**:155–164.
- [6] Cui, L., Cheng, A.H.D. and Kaliakin, V.N., 1996. Finite element analyses of anisotropic poroelasticity: a generalized Mandel’s problem and an inclined borehole problem. *Int. J. Num. Ana. Geomech.* **20**:381–401.
- [7] Hu, D.W., Zhou, H., Zhang, F. and Shao, J.F., 2010. Evolution of poroelastic properties and permeability in damaged sandstone. *Int. J. Rock Mech. Min. Sci.* **47**:962–973.
- [8] Massart, T.J. and Selvadurai, A.P.S., 2012. Stress-induced permeability evolution in a quasi-brittle geomaterial. *J. Geophys. Res. B* **117**:B07207.
- [9] Mercatoris B.C.N. and Massart T.J., 2009. Assessment of periodic homogenization-based multiscale computational schemes for quasi-brittle structural failure. *Int. J. Multiscale Comput. Engng.* **7**:153–170.
- [10] Nguyen, V.P., Lloberas-Valls, O., Stroeven, M. and Sluys, L.J., 2011. Homogenization-based multiscale crack modelling: From micro-diffusive damage to macro-cracks. *Comput. Methods Appl. Mech. Engrg.* **200**:1220–1236.