Hierarchical multiscale modeling of fluid-saturated soils

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ABSTRACT

This paper presents an extension of a hierarchical multiscale computational method previously developed by the authors to model the behavior of fluid-saturated soils. The original hierarchical multiscale framework is based on rigorous coupling between the finite element method (FEM) and the discrete element method (DEM). It helps to bypass the phenomenological constitutive assumptions needed by conventional continuum approaches. In the present study features a key extension of the framework to further consider the coupled hydro-mechanical behavior in saturated soils based on the $u-p$ formulation. It enables us to take into account the effects of pore fluid pressure and pore fluid flow on the mechanical responses of soil, while retaining reasonable computational efficiency. The approach is first benchmarked by a classic 1D consolidation problem, where the numerical predictions are compared against the closed-form solution. It is further applied to the simulation of a globally undrained biaxial compression test on a dense soil. The interplay between the fluid flow and the strain localization observed in the sample is discussed.

Keywords: hierarchical multiscale modeling, saturated soil, hydro-mechanical problem, strain localization

1 INTRODUCTION

Many catastrophic hazards in civil/geotechnical engineering, such as submarine landslides, dam failure, debris flow and earthquake liquefaction, are attributable to the presence of water (e.g. seepage flow and rainfall infiltration). Modelling a coupled hydro-mechanical system has imposed a great challenge for researchers and engineers, due to the disparately different mechanisms governing the deformation and the diffusion processes within the system.

The simplest scenario, i.e. fluid-saturated granular soil, has been commonly encountered in practice and will be considered in the study. In simulating fluid-saturated porous geomaterials, two broad categories of methods are popular nowadays. The first one is the emerging micromechanics based method, where the granular solid is treated as a collection of discrete particles using the discrete element method (DEM). But the fluid phase is still modelled as a continuum or semi-continuum with the computational fluid dynamics or the lattice Boltzmann method. Some examples applying this method include the studies of fluid-particle interactions and the debris flow (Zhao and Shan, 2013). However, this type of method is often computationally expensive. The second category of method, which treats both phases as continua, is thus prevailing in the field. The finite element method (FEM) is the most popular one among continuum-based methods due to its maturity and efficiency. When treating a coupled hydro-mechanical system, FEM has widely adopted the $u-p$ formulation (Zienkiewicz et al., 1999) to establish the governing equations (where $u$ stands for the solid displacement and $p$ is the pore fluid pressure).

In contrast to the micromechanics-based method, the continuum-based method, however, usually requires a presumed constitutive law to model the stress-strain relationship of the material. Linear elasticity is frequently adopted for simplicity. For a granular material, the constitutive response is notoriously complicated to model, involving state dependency, non-coaxiality, anisotropy and cyclic hysteresis. Many advanced models in the literature involve a good number of parameters, most of which lack clear physical meanings and are difficult to calibrate. Motivated by the issues, the hierarchical multiscale method (Guo and Zhao, 2013, 2014, 2015; Zhao and Guo, 2014) has been developed to completely abandon the phenomenological constitutive assumptions needed by conventional continuum approaches. In the
multiscale framework recently developed by the authors (Guo and Zhao, 2013, 2014, 2015; Zhao and Guo, 2014, see also Kaneko et al., 2003), the FEM is employed to discretize the problem domain and to solve the governing equations, whereas DEM packings are embedded in the Gauss points of the FEM mesh as representative volume elements (RVEs) to derive the local material responses. However, the originally proposed hierarchical multiscale method can model dry granular soils only. While the coupling effect between fluid and solid is important to a wide range of applications, the present study attempts to extend this method to address the coupled hydro-mechanical problems, based on the u–p formulation.

2 APPROACH AND FORMULATION

2.1 Governing equations

For a quasi-static problem in the absence of gravity, the balance of momentum of the fluid-solid mixture writes:

\[ \sigma_{ij,j} = 0 \quad (1) \]

where \( \sigma_{ij} \) is the total stress tensor. According to the Terzaghi’s effective stress principle, the total stress is a superposition of the effective stress \( \sigma'_{ij} \) carried by the soil skeleton and the pore fluid pressure

\[ \sigma_{ij} = \sigma'_{ij} - p\delta_{ij} \quad (2) \]

where \( \delta_{ij} \) denotes the Kronecker delta. Another equation governs the balance of mass of the fluid

\[ \left(-k_{ij}p_{ij}\right)_{i} + \frac{1}{K_f}n_i \cdot \dot{p} = 0 \quad (3) \]

where \( n \) is the porosity of the solid, \( K_f \) is the bulk modulus of the fluid, \( -k_{ij}p_{ij} = v_i \) is the Darcy velocity, and \( k_{ij} \) is the permeability tensor. In the study, we assume an isotropic permeability, i.e. \( k_{ij} = k \delta_{ij} \), where \( k \) (in the unit of \( \text{m}^2/\text{Pa} \cdot \text{s} \)) is determined from the Kozeny-Carmann equation (Andrade and Borja, 2007)

\[ k = \frac{d^3n^3}{180\mu_f(1-n)^2} \quad (4) \]

where \( d \) is the average diameter of the soil grain, \( \mu_f \) is the dynamic viscosity of the fluid.

2.2 FEM solver

Eqs. (1) and (3) can be solved by a typical FEM solver. Take the balance of momentum equation for example, it can be transformed to the matrix form upon discretization: \( K\mathbf{u} = \mathbf{R} \), where \( \mathbf{R} \) is the residual force vector, \( K \) is the global stiffness matrix, which can be assembled from the tangent modulus \( C \)

\[ K = \int_{\Omega} B^T CB d\Omega \quad (5) \]

where \( B \) is the deformation matrix, \( \Omega \) is the problem domain. For a typical nonlinear problem, \( C \) is not a constant. Newton-Raphson iteration is employed to find the converged solution. This is done by the hierarchical multiscale method, where the tangent modulus \( \mathbf{C} \) and the effective stress tensor \( \sigma'_{ij} \) are derived from the embedded DEM simulations.

2.3 DEM solver

During each Newton-Raphson iteration, the displacement gradient \( \mathbf{u}_{ij} \) is obtained at the Gauss point from the FEM solution, and is applied as the boundary condition for the corresponding DEM packing. The DEM solver will return the updated tangent modulus and the effective stress, which are homogenized from the RVE packing, respectively

\[ C_{ijkl} = \frac{1}{V} \sum_{\mathbf{c}}(k_n n_i' d_{ij} n_j' + k_t t_i' d_{ij} t_j') \quad (6) \]

\[ \sigma'_{ij} = \frac{1}{V} \sum_{\mathbf{c}} d_{ij} f_{ij} \quad (7) \]

where \( V \) is the volume of the RVE packing, \( N_c \) is the number of contacts within the packing, \( k_n \) and \( k_t \) are the normal and tangential contact stiffnesses, respectively. \( n' \) and \( t' \) are the unit vectors along the normal and tangential directions at a contact, respectively. \( d' \) and \( f' \) are the branch vector and the contact force, respectively. An illustration of these quantities is shown in Fig. 1.

Fig. 1. An illustration of the interparticle contact.

A simple linear contact law is adopted, where \( k_n \) and \( k_t \) are determined from two parameters: \( k_n = E_n r^3 \) and \( k_t = \nu c \). \( r^3 = (2r_1 r_2/(r_1 + r_2)) \) is the common radius of the two contacted particles with radii \( r_1 \) and \( r_2 \), respectively. The frictional behavior is described by the Coulomb’s criterion \( |f'| \leq \tan \phi |f_n'| \), where \( \phi \) is the interparticle friction angle.

2.4 Coupling scheme

A Gauss-Seidel-like iterative scheme is used to solve Eqs. (1) and (3) based on the “fixed-stress split” method (Kim et al., 2011). It is proved to be unconditionally stable when the implicit scheme is used.
for the time integration. The scheme can be expressed as
\[
\begin{bmatrix}
  \mathbf{u}^{(n)} \\
  p^{(n)}
\end{bmatrix}
\rightarrow
\begin{bmatrix}
  \mathbf{u}^{(*)} \\
  p^{(*)}
\end{bmatrix}
\rightarrow
\begin{bmatrix}
  \mathbf{u}^{(n+1)} \\
  p^{(n+1)}
\end{bmatrix}
\]  
(8)

where \( A^P \) and \( A^v \) are two split operators. The superscripts \((n)\) and \((n+1)\) denote two consecutive time steps. In \( A^P \), \( p \) is solved by assuming the total stress rate is constant, which yields the following relation for each iteration
\[
\varepsilon_{ij}^{(n+1,k+1)} - \varepsilon_{ij}^{(n+1,k)} = \frac{1}{K_{dr}} \left( p^{(n+1,k+1)} - p^{(n+1,k)} \right)
\]  
(9)

where \( \varepsilon_{ij} \) is the volumetric strain, the superscripts \((k)\) and \((k+1)\) denote two consecutive iterations, \( K_{dr} (= \delta_j \ C_{ijkl} \ \delta_l / 4) \) is the drained bulk modulus of the solid. The iteration of Eq. (3) can be written as
\[
\left( -k_{ij} p^{(n+1,k+1)} + \frac{n}{K_f} + \frac{1}{K_{dr}} \right) p^{(n+1,k)} = \varepsilon_{ij}^{(n+1,k)} - \varepsilon_{ij}^{(n+1,k)}
\]  
(10)

After \( p^{(n+1,k+1)} \) is updated, \( \mathbf{u}^{(n+1,k+1)} \) can be easily calculated in \( A^v \) from:
\[
\left( C_{ijkl} \varepsilon_{ij}^{(n+1,k+1)} \right) = \left( p^{(n+1,k+1)} - p^{(n)} \right)
\]  
(11)

Eq. (11) is solved by the hierarchical multiscale method. Note that there is no need to explicitly solve the intermediate displacement \( \mathbf{u}^{(*)} \) in Eq. (8) during each iteration.

3 VALIDATION

We first benchmark the implementation of the coupled hierarchical multiscale model by a classic geomechanics problem where the closed-form solution is available, namely, the Terzaghi’s 1D consolidation on an elastic soil.

3.1 RVE and material parameters

The study adopts a RVE packing containing 400 circular particles (see Fig. 2(a)) which is the same as that used in Guo and Zhao (2014). The model parameters used for the study are summarized in Table 1. Periodic boundaries are applied to both directions of the RVE. The particle radii in the RVE have been scaled 10 times larger in DEM simulations to save computational cost. So the real sand grain has a mean diameter of 0.001 m, based on which and Eq. (4) the permeability of the soil skeleton will be calculated. The packing is subjected to an initial isotropic effective stress \( \sigma_0 = 100 \) kPa and has an initial porosity \( n_0 = 0.15 \). We further assume the fluid is water with \( K_f = 2.2 \) GPa and \( \mu_f = 8.9 \times 10^{-8} \) (Pa s). The permeability can then be estimated as \( k \approx 2.9 \times 10^{-8} \) m²/(Pa s).

Table 1. Parameters for the RVE.

| Radii (mm) | Density (kg/m³) | \( E_s \) (MPa) | \( v_s \) | \( \phi \) (rad) |
|-----------|----------------|----------------|--------|-------------|
| 3–7       | 2650           | 600            | 0.8    | 0.5         |

To compare the numerical predictions with the analytical solutions, the elasticity parameters are also required. We then conduct 1D compression test on the RVE packing at small strains. The slopes of the two stress-strain lines in Fig. 2(b) give the relations \( K+4G/3 = 28 \) MPa and \( K-2G/3 = 3.7 \) MPa, where \( K \) and \( G \) are the bulk and shear moduli of the soil skeleton and are determined as \( K = 11.8 \) MPa and \( G = 12 \) MPa.

![Fig. 2. (a) RVE packing and (b) 1D compression test on the packing.](image)

3.2 1D consolidation on an elastic soil

![Fig. 3. Mesh and boundary conditions for the 1D consolidation test.](image)

A soil column with an initial height of \( H = 10 \) m is discretized with a coarse mesh using 10×1 quadrilateral elements as shown in Fig. 3. Each element contains 8 displacement nodes and 4 pressure nodes which satisfies the LBB condition to avoid the nonphysical oscillation of the pore pressure. A reduced integration scheme of 4 integration points (and hence 4 RVE packings) for each element is also used to enhance computational efficiency. The boundary conditions of the sample are prescribed by totally fixing the bottom of the column while constraining horizontal direction of...
the side boundaries to allow vertical movement. A surcharge of 110 kPa is applied on the top surface, which leads to an initial pore water pressure 10 kPa. At time \( t = 0 \), the top surface is allowed to drain while all the other boundaries are kept impervious. When the excess pore water pressure is totally dissipated, the vertical effective stress increment is 10 kPa. The soil is roughly within the elastic range seen from Fig. 2(b).

We use a non-dimensional time measure \( T \) defined as \( T = c t / H^2 \), where the coefficient of consolidation \( c \) can be estimated from the elastic moduli \( c = k/(n/K' + 1/(K+4G/3)) \approx 0.8 \). The time step \( \Delta T \) in the computation varies from 0.02 to 0.5. Fig. 4 presents the time history of the pore water pressure distribution along the column height and the degree of consolidation \( U \) defined as \( U = (u_t - u_0)/(u_0 - u_0) \), where \( u_0 \), \( u_t \) and \( u_0 \) are the immediate surface settlement, and the settlements at time \( t \) and infinite time, respectively. The analytical solutions (Verruijt and van Baars, 2007) are comparatively presented in the figure. To render better match, the coefficient of consolidation is adjusted to \( c = 0.76 \) from back-calculation, which indicates that the elastic moduli \( K+4G/3 \approx 26 \) MPa in the coupled simulation are slightly smaller than that estimated from the dry RVE test. Considering some inevitable albeit small variations of \( n, k, K \) and \( G \) in the coupled simulation due to the solid deformation, the predictions are considered as acceptable.

Fig. 4. Time history of (a) the pore water pressure distribution and (b) the degree of consolidation.

4 GLOBALLY UNDRAINED BIAXIAL COMPRESSION TEST

4.1 Mesh, boundary condition and global response

To simulate a globally undrained biaxial shear test, a specimen with a dimension of 50 mm \( \times \) 100 mm is discretized into 8\( \times \)16 quadrilateral elements shown in Fig. 5. The top and the bottom surfaces are assumed to be smooth. A uniform vertical displacement is applied on the top surface to load the specimen axially. The axial strain rate is kept constant at \( \dot{\varepsilon}_{11} = 0.001 \) s\(^{-1} \). The time step is set to \( \Delta t = 0.1 \) s. The specimen is prescribed with an initial isotropic effective stress of 100 kPa. The initial pore water pressure is uniformly set to 0. A constant confining pressure \( \sigma_{00} = 100 \) kPa is exerted on the left and the right boundaries. All the boundaries are set to be impervious to achieve the globally undrained condition, whereas local drainage is allowed by virtue of the finite permeability of the soil skeleton.

The macroscopic response of the compression test from the coupled hierarchical multiscale model is presented in Fig. 6. A dry pure DEM test on the RVE under constant volume condition is also shown for comparison. It can be seen when the strain level is small (e.g., \( \varepsilon_{11} < 0.5\% \)), the multiscale result matches the dry DEM result very well. There is a small deviation between the two when the strain becomes larger. At \( \varepsilon_{11} = 2\% \), the two temporarily coincide with each other again before totally diverging again. While the dry DEM response continues to increase afterwards, the multiscale result reaches a roughly steady state with a slight drop in the axial stress. Apparent strain localization is observed at the bifurcation point, as to be discussed in the following.

Fig. 5. Mesh and boundary condition for the biaxial compression test.

Fig. 6. Macroscopic response of the globally undrained biaxial compression test.

4.2 Strain localization and flow pattern

The contour of the porosity and the flow pattern at the four selected stages (marked in Fig. 6) are presented
in Fig. 7. Fig. 7a shows that the flow field has depicted certain localized pattern at Point A ($\varepsilon_{11}=1.49\%$) when the deformation is relatively homogeneous with a uniform porosity throughout the sample. The pattern becomes more obvious at Point B ($\varepsilon_{11}=1.6\%$). Interestingly, these two strong flow patterns occur right after the small stress drops observed at $\varepsilon_{11}=1.48\%$ and 1.59\% in Fig. 6, respectively. It indicates that when the sample strength recovers from a tiny stress drop, there appears a notable transient fluid flow. At the bifurcation point C ($\varepsilon_{11}=2.03\%$), the flow pattern still exists, but its intensity becomes rather small. When approaching the final steady state (e.g. Point D, $\varepsilon_{11}=2.39\%$), the fluid flow is vanishingly weak and the distribution of the pore water pressure within the sample is relatively uniform. A localized single shear band is unambiguously identified at the final stage of loading. Its location and inclination are coincident with the fluid flow pattern observed at the early stages of loading.

Fig. 7. Contour of porosity and flow pattern during different stages of the biaxial compression test.

It can also be seen that for a dense packing, the localized shear zone experiences dilation with high porosity, which leads to a relatively higher permeability inside the zone than that outside (c.f. Eq. (4)) and fluid flowing into the localized zone (Andrade and Borja, 2007). A striking finding is that such a flow pattern is observed much earlier than a shear band can be identified, which indicates the flow pattern can be used as a better predictor for the onset of shear band in a fluid-saturated soil.

5 CONCLUSIONS

A coupled hierarchical multiscale model was developed by extending the original single-phase multiscale model to fluid-saturated granular media based on the $u$-$p$ formulation. The model enables us to take into account the coupled effect between fluid flow and solid deformation within a hydro-mechanical system. The model was first validated by benchmarking with the classic 1D consolidation problem on an elastic soil. It was further applied to modeling the globally undrained biaxial compression test on a dense soil. Strain localization was observed in the sample with the formation of a single shear band under the smooth boundary condition. A clear correlation between the flow pattern and the shear band pattern was identified. Notable fluid flows into the dilative shear band even before the band begins to initiate, which suggests the flow pattern can be used as a better predictor for inception of strain localisation.

ACKNOWLEDGEMENTS

The study is financially supported by the Research Grants Council of Hong Kong through Project 623211.

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