A FFT-based plastic model of heterogeneous rock-like geomaterials considering micro-void evolution

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Abstract: This study focuses on the evaluation of the effective elastoplastic properties of heterogeneous rock-like geomaterials with a porous-matrix inclusion system. To investigate its effective elastoplastic properties, the material is divided into two scales. At the microscale, the porous matrix contains randomly distributed spherical micro-voids and the a solid phase, which satisfies the Drucker–Prager criterion, then, its yield behavior is described under an analytical strength-homogenization criterion of porous media. In addition, an extended evolution of micro-porosity is introduced to consider the influence of micro-void nucleation, growth, and coalescence. At the mesoscale, the material consists of a continuous porous matrix and embedded mineral inclusions. Using the two-scale heterogeneous characteristics, we develop a two-step homogenization process to determine the macroscopic mechanical properties of the material by combining with a Fast Fourier Transform-based numerical homogenization at the mesoscale and the analytical strength-homogenization method at the micro-scale. A series of numerical studies is conducted to clarify the influence of the micro-void evolution and meso inclusion on the macroscopic mechanical properties. The numerical results show that the proposed model can capture the main features of the studied geomaterial with a porous-matrix inclusion microstructure.

1. Introduction

Various types of materials such as rock, concrete, metals, and polymers are embedded with heterogeneous characteristics such as pores and inclusions at different scales. The full-field properties and effective mechanical behavior involved in the multiscale characterization of these materials can be determined using experiments to study the characteristics of the microstructure and local mechanisms at small scales [1]. They can also be estimated using analytical or computational homogenization methods to predict their effective properties [2-5].
Experimental studies have demonstrated that porous rock-like materials possess some remarkable properties, including pressure sensitivity and significant dependence on the porosity and mineralogical composition. In the perspective of micromechanics, the most common approach to strength homogenization is based on the limit analysis that employs the yield-design theory. Several theoretical models have been proposed for porous materials for a von Mises [6] or Drucker–Prager [7] solid matrix with one population of voids based on nonlinear homogenization technique, and some studies extended these works to modeling of porous materials reinforced with rigid inclusions [8]. However, the main damage mechanisms of porous materials are the growth, nucleation, and coalescence of microscopic voids in the matrix or other phase. Although a large number of predictive computational models have been proposed in the literature to provide a physical description of these mechanisms for metal materials, for example, the well-known Gurson–Tvergaard–Needleman damage model [9,10], the predictive model for two different porous-material scales with a microvoid at the microscale and meso inclusion at the mesoscale remains an open issue. This issue motivates us to investigate how the two-scale characteristics affect the macroscopic mechanical properties. Moreover, the influences of the interactions between the voids and inclusions with different microstructure physical information (inclusion shapes, sizes, orientation, and distribution) and the local stress and strain concentrations cannot be easily simultaneously considered in the criterion and limit the determination of a periodic microstructure that is statistically similar to the actual microstructure considered in this work.

To accurately estimate the overall response of heterogeneous materials, a fast Fourier transform (FFT)-based homogenization method devoted to the evaluation of physical properties for periodic-bound conditions was proposed by Moulinec and Suquet [11] to overcome the unit-cell problem of complex microstructures. Significant advancements have been achieved in various applications such as linear elastic homogenization, nonlinear elastoplastic behavior [12], and viscoplastic behavior [13]. Although this computational homogenization technique does not lead to a closed-form constitutive equation, introduction of detailed microstructural information is made possible, including the mechanical and physical geometrical properties.

In the present study, we develop a two-step homogenization process to determine the macroscopic mechanical properties of the rock-like heterogeneous geomaterial by combining it with the FFT-based numerical homogenization at the mesoscale and the analytical strength-homogenization method at the microscale. An extended evolution of microporosity is also proposed to consider the influence of microvoid nucleation, growth, and coalescence. Using the two-step homogenization process, a series of numerical studies is conducted to clarify the influence of microvoid evolution and meso inclusion on the macroscopic mechanical properties.

2. Basic formulation of microstructure at three scales

For the micromechanical modeling, the representative volume element (RVE) is first defined. Let us consider a periodic geomaterial composed of a large number of RVEs or unit cells that display three-scale heterogeneous characteristics. Each unit cell can be regarded as a composite with pores and mineral inclusions embedded in two separate scales, as shown in Figure 1. At the mesoscale, the microstructure is characterized by a porous matrix and mineral inclusion. At the microscale, the matrix is a porous medium composed of solid particles and arbitrarily distributed inter-particle pores inside. Its pore size is much smaller than that in the mineral inclusion. For
simplicity, we assume that the pores at the microscale are spherical and isotopically arranged, whereas the inclusion at the mesoscopic scale is regarded as an elastic material and can be assumed to have various geometries and distributions. Let us denote the total volume of the studied unit cell as \( \Omega \), the domain occupied by the solid phase at the microscopic scale as \( \omega_m \), and the volumes of the pores located at the microscopic and inclusions at the mesoscopic scales as \( \omega_1 \) and \( \omega_2 \), respectively. In these expressions, porosity \( f \) at the microscale, volume fraction \( \rho \) of the inclusions at the mesoscale, and total porosity \( \Gamma \) at the macroscale can be expressed as

\[
f = \frac{\omega_1}{\omega_m + \omega_1}, \quad \rho = \frac{\omega_2}{\omega_m + \omega_1 + \omega_2}, \quad \Gamma = \frac{\omega_1}{\omega_m + \omega_1 + \omega_2}
\]

To investigate the macroscopic behavior of the three-scale materials, a two-step upscaling is adopted in this study for the transitions from microscale to mesoscale and from mesoscale to macroscale. In the first homogenization, the microvoids and property of the solid phase are considered. The effect of the meso inclusion on the overall behavior is considered in the second homogenization using the FFT technique. The process is presented in detail in the next sections.

2.1 Upscaling from microscale to mesoscale

Compared with that of metal materials, pressure sensitivity represents the main characteristics of a geomaterial. To consider the plastic compressibility of the matrix, the solid phase is assumed to satisfy a Drucker–Prager-type criterion, i.e.,

\[
F_m = \sigma_{eq} + 3\alpha \sigma_m - \sigma_0
\]

where \( \sigma \) denotes the microscopic stress tensor, \( \sigma_0 \) represents the yield stress of the matrix, and \( \sigma_m = tr\sigma/3 \) denotes the mean stress. The von Mises equivalent stress is defined as \( \sigma_{eq} = \sqrt{\frac{1}{2} \sigma : \sigma} \), where \( \sigma' \) is the deviatoric part of the stress tensor. Parameter \( \alpha \) represents the pressure-sensitivity coefficient, which is physically related to the internal friction angle of solid matrix \( \varphi \) by \( \tan \varphi = 3\alpha \).

Figure 1(c) shows that the porous matrix contains a Drucker–Prager type matrix and is configured with spherical voids. To describe its homogenized mechanical properties, a strength-yield criterion was derived by Shen et al. (2016) in the framework of kinematical limit-analysis theory, which is expressed as follows:
The criterion in Eq. (3) depends on porosity $f$ at the microscopic scale and pressure-sensitive parameter $\alpha$ of the solid phase. This criterion is adopted in the first homogenization from microscale to mesoscale to consider the influence of microporosity and plastic compressibility in the solid phase. We must note that $\Sigma$ represents the mesostress of the porous matrix at the mesoscopic scale [Figure 1(b)], and that at the macroscopic scale is denoted as $\Sigma$ [Figure 1(a)].

Total strain rate $\dot{\mathbf{D}}$ of the porous matrix is further divided into elastic part $\dot{\mathbf{D}}^e$ and plastic part $\dot{\mathbf{D}}^p$. The effective stress–strain relationship of the porous matrix can be expressed in the following incremental form:

$$\dot{\mathbf{D}} = \dot{\mathbf{D}}^e + \dot{\mathbf{D}}^p, \dot{\Sigma} = \mathbf{C}_m \mathbf{D} \dot{\Sigma} - \mathbf{C}_m \mathbf{D} \dot{\Sigma} = \mathbf{C}_m (\mathbf{D} - \mathbf{D}^p) \tag{4}$$

where $\mathbf{C}_m$ is the effective elastic stiffness tensor of the porous matrix. By assuming an isotropic material, $\mathbf{C}_m$ can be expressed as $\mathbf{C}_m = 3k_0^{hom} \mathbf{I} + 2\mu_0^{hom} \mathbf{I}$, where $\mathbf{I}_{ijkl} = \delta_{ij}\delta_{kl}/3$, $\mathbf{I}_{ijkl} = \mathbf{I}_{ijkl} - \mathbf{I}_{ijkl}$, and $\mathbf{I}_{ijkl} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$. Here, $\delta_{ij}$ is the Kronecker symbol. $k_0^{hom}$ and $\mu_0^{hom}$ are the effective bulk and shear moduli of the porous matrix, respectively, which are dependent on the porosity and bulk and shear moduli ($k_s$ and $\mu_s$) of the solid phase. In the present study, it is determined using the Mori–Tanaka scheme (Mori and Tanaka, 1973), which corresponds to the Hashin–Shtrikman upper bound (Hashin and Shtrikman, 1963).

$$k_0^{hom} = \frac{4(1-f)k_s\mu_s}{4\mu_s + 3f k_s}, \mu_0^{hom} = \frac{(1-f)\mu_s}{1 + 6f \frac{\beta_\mu}{\delta + 9k}} \tag{5}$$

To consider the plastic-hardening behavior, the frictional coefficient is assumed to evolve with the equivalent plastic strain. Thus, the following form is used:

$$\dot{\mathbf{D}}^p = d\lambda \frac{\partial F}{\partial \Sigma} \tag{6}$$

We assume that the porous matrix exhibits elastoplastic behavior. The plastic deformation of the porous matrix is further described by an associated plastic-flow rule. Therefore, the plastic-strain rate of the porous matrix is given by

$$\alpha = \alpha_m - (\alpha_m - \alpha_0)e^{-ks_e^p}, \tag{7}$$

where variable $e^p$ denotes the equivalent plastic strain of the matrix. Its evolution can be expressed as

$$e^p = \frac{\Sigma \cdot \dot{D}^p}{(1-f)\sigma_0} \tag{8}$$

Generally, the evolution of a micro-void is caused by two contributions: void growth $\dot{f}_g$ and void nucleation $\dot{f}_n$. Thus, $\dot{f} = \dot{f}_g + \dot{f}_n$. The void growth is assumed to be due to the incompressibility of bulk materials under plastic deformation. Its detailed derivation can be found in the work of Cao et al. (2018), who used the kinematical compatibility condition, i.e.,

$$\dot{f}_g = (1-f)(\text{tr} D^p - a e^p) \tag{9}$$
To describe the nucleation of new micro-voids, the stress or strain of its porosity evolution must be controlled. A widely used strain-controlled void-nucleation law is considered to follow a normal distribution, as proposed by Chu and Needleman (1980).

\[
\dot{f}_n = A_N \dot{\varepsilon}^\beta \text{ with } A_N = \frac{f_N}{S_N \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon^p - \varepsilon_N}{S_N} \right)^2 \right]
\]

where \( f_N \) is the maximum potential nucleated-void volume fraction relative to the volume fraction of the second phase that allows the nucleation. \( \varepsilon_N \) and \( S_N \) are material parameters. According to the work of Tvergaard and Needleman (2008), the effect of the void coalescence is considered by replacing Eq. (3) with effective porosity \( f^* \). Then, the effect can be numerically simulated using an artificially accelerated void growth defined by the following bilinear function:

\[
f^* = \begin{cases} 
  f & \text{for } f \leq f_c \\
  f_c + \frac{f_u - f_c}{f_f - f_c} f & \text{for } f > f_c
\end{cases}
\]

where \( f_u \) is the ultimate value of \( f^* \) at the occurrence of ductile rupture, \( f_c \) is the critical void-volume fraction at the onset of coalescence, and \( f_f \) is the porosity at the final failure. The objective of \( f^* \) is to model the complete disappearance of the load-carrying capacity due to void coalescence.

### 2.2 Upscaling from mesoscale to macroscale

In the first homogenization step from microscale to mesoscale, micro-porosity \( f \) in the porous matrix is considered in the analytical yield criterion, namely, Eq. (3). In the current work, the FFT technique proposed by Moulinec and Suquet (1994) can well capture the geometry of the inclusions at the mesoscopic scale for the second homogenization step. The basic framework of the FFT technique for a nonlinear mechanical problem is recalled in detail.

We first consider a unit cell of an inhomogeneous material subjected to macroscopic strain tensor \( \varepsilon \) under periodic boundary conditions. The studied material has local stiffness \( C(x) \). Then, the unit cell is discretized into a regular grid consisting of \( N \times N \times N \) voxels corresponding to each coordinate point \( x \) in real space. For an elastoplastic material, the local problem can be expressed as

\[
\begin{cases} 
  \Delta \sigma(x) = C_{\text{trans}}(x) : \Delta \varepsilon(x) \\
  \text{div} \sigma(x) = 0 & \forall x \in \Omega, u^* \in \mathbb{R}^N, \sigma \cdot n = 0 & \forall \partial \Omega \\
  \varepsilon(x) = \frac{1}{2} (\mathbf{u}^*(x) + \mathbf{u}^*(x)) + \mathbf{E} \cdot \mathbf{x} \Omega
\end{cases}
\]

This local problem can be reduced into a periodic Lippmann–Schwinger equation by introducing periodic Green operator \( \Gamma_0 \) associated with reference stiffness tensor \( C_0 \) and polarization tensor field \( \mathbf{r}(x) = (C(x) - C_0) : \varepsilon(x) \). The solution of this local problem in the Fourier space can be expressed as

\[
\mathbf{\hat{r}}(\xi) = -\mathbf{\hat{r}}^0(\xi) \cdot \mathbf{\hat{r}}(\xi) \forall \xi \neq 0, \mathbf{\hat{r}}(0) = \mathbf{E}
\]

where \( \mathbf{\hat{r}}(\xi) \) and \( \mathbf{\hat{r}}^0(\xi) \) are the polarization tensor and periodic Green operator in the Fourier space at each discrete frequency \( \xi \), respectively. The Green operator in the Fourier space can be expressed as

\[
\Gamma_{ijkl}(\xi) = \frac{1}{4 \mu_0 \xi^2} \left( \delta_{ik} \delta_{jl} + \delta_{ik} \delta_{jl} + \delta_{ij} \delta_{lk} + \delta_{ij} \delta_{lk} \right) - \frac{\lambda_0 + 2 \mu_0}{\mu_0 (\lambda_0 + 2 \mu_0)} \frac{\xi_i \xi_j \xi_k \xi_l}{\left| \xi \right|^4}
\]

Accordingly, the FFT-based iterative process for nonlinear heterogeneous materials at loading...
step \( n + 1 \) is defined by the following algorithm:

**Algorithm**:

Initialization: \( \varepsilon^{(n+1)0}(x) = \varepsilon^n(x) + \Delta \varepsilon^{n+1} \)

Call the elastoplastic subroutine to calculate \( C^{\text{strain}}(n+1)^0(x_p,V^{(n+1)^0}) \)

\( \sigma^{(n+1)0}(x) = \sigma^n(x) + C^{\text{strain}}(n+1)^0(x_p); \Delta \varepsilon^{(n+1)0}(x_p) \forall x_p \in \Omega \)

Iterate \( i + 1 \):

The previous \( \varepsilon^n \) and \( \sigma^n \) are known at each position \( x_p \)

\( a) \quad \varepsilon^{(i+1)^0} = \mathcal{F} \mathcal{F}^{-1}(\sigma^i) \);  
\( b) \quad \text{Verify the convergence and update the stress/strain} \);  
\( c) \quad \varepsilon^{(i+1)^0}(x_p) = \varepsilon^i(x_p) - I^i(x_p) \sigma^i(x_p); \sigma^i(x_p) \);  
\( d) \quad \varepsilon^{(i+1)^0} = \mathcal{F} \mathcal{F}^{-1}(\sigma^{(i+1)^0}) \);  
\( e) \quad \text{Call the elastoplastic constitutive relation to calculate } C^{\text{strain}}(i+1)(x_p,V^{(i+1)}) \);  
\( f) \quad \text{update stress tensor } \sigma^{i+1}(x) = \sigma^n(x) + C^{\text{strain}}(i+1)(x_p); \Delta \varepsilon^{(i+1)}(x_p) \forall x_p \in \Omega \);  
\( g) \quad \text{Conserve internal variable } V^{i+1} \)

3. Numerical simulations of the elastoplastic behavior of the studied material

This section presents the series of numerical experiments performed to investigate the macroscopic mechanical properties of the studied multiscale rock-like geomaterial using the proposed two-step homogenization process. The influences of the micro-void and meso inclusion on the macroscopic mechanical response are analyzed and presented in detail.

3.1 Evolution of macroscopic plastic failure surface

We first consider a unit cell that contains a porous matrix and a centrally located spherical inclusion with different volume fractions of micro-void and meso inclusion. To derive the evolution of the macroscopic plastic failure surface in the \( \Sigma_m - \Sigma_{eq} \) plane, the mechanical behavior of the porous matrix is assumed to be perfect elastoplastic. Thus, the plastic-hardening and microvoid evolution are both ignored in this case. The material parameters of the solid phase in the porous matrix are presented as follows: \( E_s = 5 \) GPa, \( \nu_s = 0.15, \alpha = 0.1, \) and \( \sigma_0 = 10 \) MPa. Here, the spherical inclusion is assumed to be elastic, and its Young’s modulus and Poisson’s ratio are chosen as \( E_i = 98 \) GPa and \( \nu_i = 0.15, \) respectively.

![Figure 2](image-url)  

**Figure 2.** Computation of the effective yield surfaces at different micro-porosity and volume-fraction values of the meso inclusion.

Figure 2 shows the computed yield-surface evolution at different constituent porosities and volume fractions of the inclusion. We can observe that at a lower micro-porosity or higher
inclusion volume fraction, the failure strength of the studied material is significantly enhanced. In addition, the macroscopic yield surfaces are unsymmetrical in the compression and tension regions for a composite unit cell with a Drucker-Prager type solid phase. Comparison of the yield surfaces at different volume fractions of the inclusions shows that the inclusion content is insensitive to the yield strength in the case of hydrostatic loading, especially under tension condition. Meanwhile, porosity plays a more important role in the yield-surface evolution [Figure 2(b)] in the compression region than in the tension region.

3.2 Evolution of the macroscopic stress–strain curves

In the context of the present work, our interest in rock-like materials is determining how the micro-void and meso inclusion affect its macroscopic stress–strain curves. For the studied unit cell, the elastic parameters of the matrix and inclusion are the same as those mentioned in the previous Section 3.1. The plastic-material parameters are listed in Table 1.

| $a_0$ | $a_m$ | $b$ | $\sigma_0$ (MPa) | $F_N$ | $S_N$ | $\varepsilon_N$ | $f_{\alpha}$ | $f_f$ | $f_c$ |
|-------|-------|-----|-----------------|-------|-------|----------------|------------|-------|-------|
| 0.1   | 0.25  | 500 | 10              | 0.4   | 0.1   | 0.4            | 0.7        | 0.25  | 0.12  |

(a) Stress – strain relation with $f = 0.1$

(b) Microporosity evolution

Figure 3. Modeling results of the macroscopic stress–strain curves under the uniaxial compression test for a unit cell with different inclusion fractions and the evolution of their average microporosity.

(a) Stress – strain relation with $\rho = 0.1$

(b) Microporosity evolution

Figure 4. Modeling results of macroscopic stress–strain curves under uniaxial compression test for the unit cell with different micro-porosity and their evolution of average microporosity.
micro-porosity.

By using the proposed two-step homogenization process, a series of numerical simulations under uniaxial compression test is conducted for a unit cell with different micro-porosity and volume fractions of meso inclusions. Figures 3 and 4 show the evolution of the macroscopic stress–strain curves and average micro-porosity of the unit cell, respectively, at different inclusion fractions and micro-porosity. We can clearly observe that a higher inclusion fraction can enhance the failure strength. In contrast, the micro-void exerts a significantly weaker effect. In addition, the post-failure softening behavior is well captured.

4. Conclusions

In this work, to estimate the effective elastoplastic properties of heterogeneous rock-like geomaterials with a porous-matrix inclusion system, a two-step homogenization procedure is developed by combining the analytical homogenization method and FFT-based computational homogenization technique. A microvoid evolution function is introduced to describe the void growth, nucleation, and coalescence. As demonstrated by the numerical tests, the proposed model successfully captures the main influences of the heterogeneous characteristics such microvoid and inclusion on the damage behavior of the porous-matrix inclusion microstructure.

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