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# A micro-mechanical constitutive model for heterogeneous rocks with non-associated plastic matrix as implicit standard materials

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## Abstract

In this work, we shall propose a new micro-mechanical constitutive model for the estimation of effective elastic-plastic behaviors of heterogeneous rocks. A bi-potential based incremental variational (BIV) approach is developed in order to take into account non-uniform local strain fields of constituents. The studied materials are composed of a non-associated and pressure sensitive plastic matrix, elastic inclusions and/or voids. For clarity, the local behavior of matrix is first described by an elastic perfectly-plastic model. Based on the bi-potential theory to dealing with non-associated plastic flow, the solid matrix is considered as pertaining to implicit standard materials (ISMs). The effective incremental bi-potential and macroscopic stress tensor are then estimated through an extension of the incremental variational method initially established for generalized standard materials (GSMs). The accuracy of the BIV model is verified by comparing the model's predictions with the reference results obtained from direct finite element simulations. Furthermore, by assuming that the general formulation obtained for the perfectly plastic matrix remains valid for each loading increment, the BIV model is extended to considering that the solid matrix exhibits an isotropic hardening by using an explicit algorithm. The accuracy of the extended BIV model is also validated by a series of comparisons with the reference solutions obtained by direct finite element simulations for both inclusion-reinforced composites and porous materials. Both local and macroscopic responses are compared. As an example of application, the extended BIV model is finally applied to estimating the mechanical responses of typical claystone and sandstone under different loading paths.

**Keywords:** Micro-mechanics, Nonlinear homogenization, Non-associated plasticity, Heterogeneous rocks, Claystone, Sandstone

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## 1. Introduction

Rocks are usually regarded as typical composites, which are used in a very wide range of engineering constructions. These materials contain different kinds of heterogeneities at different scales. Pores and inclusions are two main families of heterogeneities. Furthermore, these materials are composed of several mineral phases of different properties. The mineral compositions may significantly vary in space, for instance with geological depth. Laboratory studies have shown that the macroscopic physical and mechanical properties of these materials are affected by heterogeneities and mineral compositions. So far, different kinds of macroscopic models, mainly elastic-plastic and damage models have been developed. Directly fitted from laboratory tests, these models are able to correctly reproduce the main features of mechanical behaviors of those materials. However, they are not able to properly consider the effect of heterogeneities and mineralogical compositions on the macroscopic mechanical responses.

Based on linear homogenization techniques, micro-mechanical models have first been established during the last decades for modeling induced damage in brittle rocks (Zhu et al., 2008, 2016, Zhao et al., 2018, Zhang et al., 2019). Important advances have also been obtained on micro-mechanical modeling of plastic deformation in ductile and porous rocks by using nonlinear homogenization methods. For instance, clayey rocks have been characterized as composites constituted of a plastic clay matrix in which calcite and quartz grains are embedded (Guéry et al., 2008, Jiang et al., 2009). In some multi-scale models, the microstructure of clayey rocks has further been enriched by considering the clay matrix as a porous material at the microscopic scale (Shen et al., 2012). The effective inelastic behavior of the porous clay matrix has been estimated by using the Hill incremental method (Hill, 1965). As for metallic composite materials, it was found that the use of the original Hill's incremental method produced too stiff mechanical behaviors (Suquet, 1996, Chaboche et al., 2005). The main reason is the fact that uniform local strain fields are assumed in constituents of composites in the Hill's method. In order to improve the numerical performance of this method, artificial techniques, such as isotropization of tangent elastic-plastic stiffness tensor, have been proposed. This correction technique has also been applied to clayey rocks (Guéry et al., 2008, Jiang and Shao, 2009, Shen et al., 2012). However, all those correction techniques are generally not based on any physical background.

Meanwhile, advanced nonlinear homogenization techniques have been developed for composite materials considering non-uniform local fields in constituent phases (Castañeda, 1991, 1992, 2002, Lahellec and Suquet, 2007a,b, 2013, Boudet et al., 2016, Brassart et al., 2011, 2012, Danas and Castañeda, 2012), just to mention some representative ones. In particular, variational principles based

33 on the use of a "linear comparison composite (LCC)" were proposed for the mean field homoge-  
34 nization method of nonlinear elastic composites (Castañeda, 1991, 1992, 2002), and used to generate  
35 improved bounds and more generate estimates for the nonlinear elastic-plastic composites (Castañeda  
36 and Suquet, 1997, Danas and Castañeda, 2012). By extending these previous works, a new incremen-  
37 tal variational method has been established (Lahellec and Suquet, 2007a,b) for modeling effective  
38 nonlinear properties of viscoelastic composites without local threshold or hardening. In this new  
39 method, equivalent interval variables (EIV) are introduced to capture the non-uniform local plastic  
40 strain fields. Further, the same authors have proposed a rate variational model (RVP) by considering  
41 a non-uniform field of plastic strain rate (Lahellec and Suquet, 2013). More recently, the EIV method  
42 has been extended to modeling elastic-(visco)plastic composites with local threshold and isotropic  
43 and/or linear kinematic hardening (Boudet et al., 2016). On the other hand, based on the variational  
44 principle established in Ortiz and Stainier (1999), alternative incremental variational models have  
45 been proposed in Brassart et al. (2011, 2012) for studying elastic-(visco)plastic composites with lo-  
46 cal isotropic hardening. The EIV method has further been extended to the description of geological  
47 materials with a pressure-dependent Drucker-Prager plastic matrix (Zhao et al., 2019). However, all  
48 these previous models have been developed in the scope of Generalized Standard Materials (GSMs)  
49 (Halphen and Nguyen, 1975) with an associated plastic flow rule.

50 Extensive experimental results have clearly shown that for most rocks, a non-associated plastic  
51 flow rule is required for correctly modeling the coupling between shear and volumetric strains. These  
52 materials cannot be considered as Generalized Standard Materials. As a first approximation, the  
53 microstructure of these materials at a selected relevant length scale, for instance micrometer, can be  
54 characterized by the representative unit cell shown in Figure 1. Several sets of elastic inclusions  
55 (mineral grains in rocks) are embedded in a plastic matrix (clay matrix in clayey rocks). The local  
56 behavior of the matrix is generally described by a non-associated and pressure sensitive plastic model.  
57 The incremental variational methods developed for the GSMs cannot be directly used to estimate the  
58 effective mechanical behaviors of rocks.

59 In order to generalize the incremental variational principles to heterogeneous rocks, the idea here  
60 is first to transform these non-GSMs into a class of implicit standard materials (ISM). This is done  
61 with the help of the bi-potential theory initially developed for macroscopic elastic and plastic behav-  
62 iors of non-GSMs (De Saxcé and Feng, 1991, De Saxcé and Bousshine, 1998, De Saxcé, 1995). This  
63 theory has been successfully used for modeling soils and rock-like materials with non-associated plas-  
64 tic models (Bodovillé and De Saxcé, 2001, Bodovillé, 2001, Hjiiaj et al., 2003, Berga, 2012). More-

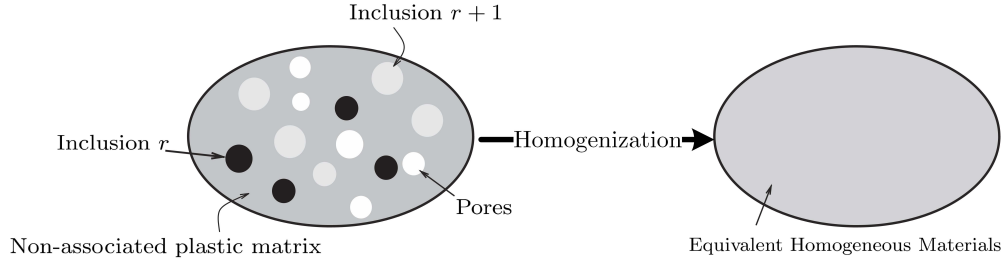


Figure 1: Representative volume element (RVE) of heterogeneous rocks at a selected length scale

65 over, the bi-potential theory is naturally suitable for developing a variational approach of constitutive  
 66 modeling.

67 With the help of the bi-potential theory, the aim of this work is to develop a new incremental  
 68 variational method for estimating the effective elastic-plastic behavior of heterogeneous rocks com-  
 69 posed of a non-associated and pressure sensitive plastic matrix. This is based on the construction of  
 70 an incremental elastic-plastic bi-potential for ISMs by using an implicit time-discretization scheme.

71 On the other hand, ductile and porous heterogeneous rocks generally exhibit plastic hardening.  
 72 For instance, in the case of an isotropic hardening, the internal friction or cohesion can evolve during  
 73 plastic deformation. In the case of heterogeneous rocks idealized in Figure 1, plastic hardening oc-  
 74 curs in the plastic matrix. This mechanism should be taken into account. However, the formulation  
 75 of an incremental variational model for materials with a pressure-sensitive plastic matrix with plastic  
 76 hardening may becomes mathematically very complex. By taking the incremental nature of the ap-  
 77 proach, a simplified explicit method is proposed in this paper. The new bi-potential base incremental  
 78 variational model (BIV) is first developed by considering a perfectly plastic matrix. Then at the end  
 79 of each loading increment, the plastic properties are updated but frozen for next loading increment.  
 80 The plastic matrix is then considered as a material without hardening during the current increment.

81 The proposed new BIV model is validated by comparing model's predictions and numerical results  
 82 issued from direct finite element simulations for both perfectly plastic and plastic with hardening  
 83 cases. Finally, the new BIV model is applied to estimating the effective mechanical responses of  
 84 typical claystone and porous sandstone in various loading paths.

85 Throughout this paper, the following notions of tensorial products of any second order tensors  $\mathbf{A}$   
 86 and  $\mathbf{B}$  will be used:  $(\mathbf{A} \otimes \mathbf{B})_{ijkl} = A_{ij}B_{kl}$  and  $\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}$ . Fourth order tensors are denoted by  
 87 blackboard bold characters, and one can define  $(\mathbb{C} : \mathbf{B})_{kl} = C_{ijkl}B_{kl}$ . The symbol  $\|\mathbf{A}\| = \sqrt{\mathbf{A} : \mathbf{A}}$  is  
 88 used to denote the norm of any second order tensor  $\mathbf{A}$ . With the second order identity tensor  $\delta$ , usually  
 89 used fourth order isotropic identity tensor  $\mathbb{I}$  and fourth order hydrostatic projects  $\mathbb{J}$  are expressed in

90 the components form as  $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$  and  $J_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}$ , respectively. The fourth order  
 91 deviatoric projects  $\mathbb{K} = \mathbb{I} - \mathbb{J}$  is then obtained. Moreover, the fourth-order tensors  $\mathbb{J}$  and  $\mathbb{K}$  have the  
 92 properties:  $\mathbb{J} : \mathbb{J} = \mathbb{J}$ ,  $\mathbb{K} : \mathbb{K} = \mathbb{K}$ ,  $\mathbb{J} : \mathbb{K} = \mathbb{K} : \mathbb{J} = \mathbf{0}$ .

## 93 2. Bi-potential theory for non-associated plastic flow rule

### 94 2.1. Generalized standard materials (GSM)

95 A large class of solid materials can be described by using a generalized framework based on  
 96 the existence of two convex potentials conjugating one to the other  $V(\dot{\boldsymbol{\varepsilon}})$  and  $W(\boldsymbol{\sigma})$  satisfying the  
 97 Fenchel's inequality (Fenchel, 1949)

$$\forall (\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \quad W(\boldsymbol{\sigma}) + V(\dot{\boldsymbol{\varepsilon}}) \geq \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \quad (1)$$

98 where  $\boldsymbol{\sigma}$  is the Cauchy stress tensor and  $\dot{\boldsymbol{\varepsilon}}$  is the strain rate tensor. A pair of  $(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}})$  is said to be  
 99 extremal if the equality is achieved, that is:

$$W(\boldsymbol{\sigma}) + V(\dot{\boldsymbol{\varepsilon}}) = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \quad (2)$$

100 Then, any extremal pair is characterized by the following relations:

$$\forall \boldsymbol{\sigma}' \quad W(\boldsymbol{\sigma}') - W(\boldsymbol{\sigma}) \geq (\boldsymbol{\sigma}' - \boldsymbol{\sigma}) : \dot{\boldsymbol{\varepsilon}} \quad (3a)$$

$$\forall \dot{\boldsymbol{\varepsilon}}' \quad V(\dot{\boldsymbol{\varepsilon}}') - V(\dot{\boldsymbol{\varepsilon}}) \geq \boldsymbol{\sigma} : (\dot{\boldsymbol{\varepsilon}}' - \dot{\boldsymbol{\varepsilon}}) \quad (3b)$$

101 Therefore,  $\boldsymbol{\sigma}$  and  $\dot{\boldsymbol{\varepsilon}}$  are expressed by the sub-differential mappings

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial \dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\varepsilon}}), \quad \dot{\boldsymbol{\varepsilon}} = \frac{\partial V}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}) \quad (4)$$

102 These relations constitute the normality rule. Different kinds of constitutive equations, such as plastic  
 103 laws, visco-plastic law and plastic hardening laws can generally and conveniently be constructed with  
 104 Eq.(4). The class of materials governed by the two convex potentials are called generalized standard  
 105 materials (GSMs) (Halphen and Nguyen, 1975).

### 106 2.2. Implicit standard material

107 However, the mechanical behavior of a large number of materials cannot be integrated within the  
 108 above framework. For example, for most heterogeneous rocks, one of the constituent phase exhibits  
 109 a plastic or viscoplastic behavior which is generally described by a non-associated flow rule. The  
 110 normality rule is then not verified. Conventional approaches for modeling the non-associated plastic

111 deformation are based on the choice of two independent functions of stress tensor, the plastic yield  
 112 function to determine yield locus and the plastic potential function giving the plastic strain evolution  
 113 law. However, this type of approaches loses the good property of convexity (De Saxcé, 1995, Berga,  
 114 2012). The bi-potential theory proposed by De Saxcé and Feng (1991) provides a convenient math-  
 115 ematical frame for dealing with non-associated plastic materials. It allows keeping the key-concept  
 116 of normality and convexity. This theory generalizes the Fenchel's inequality to materials and systems  
 117 with non-standard behaviour. To find the concept of normal dissipation, the constitutive laws are for-  
 118 mulated under an implicit form. For the sake of clarity, the basic notion of implicit standard materials  
 119 (ISMs) is here recalled (De Saxcé and Feng, 1991).

120 For describing the behaviour of ISMs, a bi-potential  $b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}})$  is first introduced. It is a scalar-  
 121 valued function, convex with respect to  $\boldsymbol{\sigma}$  when  $\dot{\boldsymbol{\varepsilon}}$  keeps constant, and convex with respect to  $\dot{\boldsymbol{\varepsilon}}$  when  
 122  $\boldsymbol{\sigma}$  remains constant. The bi-potential function should also verify the following inequality

$$\forall (\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \quad b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \geq \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \quad (5)$$

123 If and only if the pair  $(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}})$  is obtained at the extreme value, implying that  $(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}})$  satisfies the consti-  
 124 tutive relation of the material, one has

$$b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \quad (6)$$

125 Then, any extremal pair is characterized by the following relations:

$$\forall \boldsymbol{\sigma}' \quad b(\boldsymbol{\sigma}', \dot{\boldsymbol{\varepsilon}}) - b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \geq (\boldsymbol{\sigma}' - \boldsymbol{\sigma}) : \dot{\boldsymbol{\varepsilon}} \quad (7a)$$

$$\forall \dot{\boldsymbol{\varepsilon}}' \quad b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}') - b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \geq \boldsymbol{\sigma} : (\dot{\boldsymbol{\varepsilon}}' - \dot{\boldsymbol{\varepsilon}}) \quad (7b)$$

126 Accordingly,  $\boldsymbol{\sigma}$  and  $\dot{\boldsymbol{\varepsilon}}$  are related by the subnormality laws

$$\boldsymbol{\sigma} = \frac{\partial b}{\partial \dot{\boldsymbol{\varepsilon}}}(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}), \quad \dot{\boldsymbol{\varepsilon}} = \frac{\partial_{\boldsymbol{\sigma}} b}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) \quad (8)$$

127 These relations provide a multi-valued constitutive relationship between  $\boldsymbol{\sigma}$  and  $\dot{\boldsymbol{\varepsilon}}$ , which is now im-  
 128 plicit in the sense of the implicit function theorem. It is noted that GSMs can be considered as  
 129 particular cases of ISMs with separable bi-potentials:

$$b(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}) = W(\boldsymbol{\sigma}) + V(\dot{\boldsymbol{\varepsilon}}) \quad (9)$$

### 130 2.3. Incremental elastic-plastic bi-potential

131 We consider now the local elastic-plastic behavior of the solid matrix in heterogeneous rocks. For  
 132 the sake of clarity, the behavior of matrix is described by an elastic perfectly plastic non-associated

133 model. Under the assumption of isothermal conditions and small strains, the total strain tensor  $\boldsymbol{\varepsilon}$  is  
 134 decomposed into an elastic part  $\boldsymbol{\varepsilon}^e$  and a plastic one  $\boldsymbol{\varepsilon}^p$

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p \quad (10)$$

135 In view of applying the incremental variational method to determining the effective mechanical be-  
 136 havior of heterogeneous rocks, it is needed to derive an incremental elastic-plastic bi-potential for  
 137 the plastic matrix. To this end, the general forms of the elastic and plastic bi-potentials are first sep-  
 138 arately formulated. Then the incremental elastic-plastic bi-potential is established by using a time-  
 139 discretization scheme.

### 140 2.3.1. Elastic bi-potential

141 In the elastic regime, the bi-potential conforms to the characteristics of GSMs. Moreover, the  
 142 elastic laws can be derived from the strain energy density function  $V(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p)$  and the complementary  
 143 energy density function  $W(\boldsymbol{\sigma})$ . Therefore, the elastic bi-potential  $b_e$  is a separate function with the  
 144 following expression

$$b_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) = V(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + W(\boldsymbol{\sigma}) \quad (11)$$

145 which satisfies the implicit standard laws

$$\boldsymbol{\sigma} = \frac{\partial b_e}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) = -\frac{\partial b_e}{\partial \boldsymbol{\varepsilon}^p}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \quad \text{and} \quad \boldsymbol{\varepsilon} = \frac{\partial b_e}{\partial \boldsymbol{\sigma}}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) + \boldsymbol{\varepsilon}^p \quad (12)$$

### 146 2.3.2. Plastic bi-potential

147 Under the plastic state, the non-associated plastic model falls into the category of ISMs. By virtue  
 148 of (5) the plastic bi-potential function is first defined by the condition:

$$\forall (\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) \quad b_p(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) \geq \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p \quad (13)$$

149 Similarly, if and only if the pair  $(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p)$  reaches the extreme value, one gets:

$$b_p(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p \quad (14)$$

150 Then  $\boldsymbol{\sigma}$  and  $\dot{\boldsymbol{\varepsilon}}^p$  are related by subnormality laws:

$$\boldsymbol{\sigma} = \frac{\partial b_p}{\partial \dot{\boldsymbol{\varepsilon}}^p}(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p), \quad \dot{\boldsymbol{\varepsilon}}^p = \frac{\partial b_p}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) \quad (15)$$



### 151 2.3.3. Incremental elastic-plastic bi-potential

Combining Eqs. (12) and (15), the constitutive relations of the plastic phase under consideration can be expressed as a system of two coupled equations, one of them being a differential equation in time:

$$\sigma = \frac{\partial b_e}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \quad (16a)$$

$$\frac{\partial b_e}{\partial \boldsymbol{\varepsilon}^p}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) + \frac{\partial b_p}{\partial \dot{\boldsymbol{\varepsilon}}^p}(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) = 0 \quad (16b)$$

152 Based on the previous work by [Ortiz and Stainier \(1999\)](#), the time derivative  $\dot{\boldsymbol{\varepsilon}}^p$  is approximated by  
 153 a difference quotient after the use of an implicit Euler-Scheme. The whole time period (whole loading  
 154 history) of study  $[0, T]$  is accordingly divided into the time steps (loading steps)  $t_0 = 0, t_1, \dots, t_n, t_{n+1}, \dots, t_N =$   
 155  $T$ . The time increment between  $t_n$  and  $t_{n+1}$  (loading increment) is denoted by  $\Delta t$ . For the sake of sim-  
 156 plifying the notations, its dependence on  $n$  is omitted. By using this time-discretization scheme, the  
 157 system of differential equations (16) is transformed to the following discretized system:

$$\sigma_{n+1} = \frac{\partial b_e}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\varepsilon}_{n+1}^p, \boldsymbol{\sigma}_{n+1}), \quad \frac{\partial b_e}{\partial \boldsymbol{\varepsilon}^p}(\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\varepsilon}_{n+1}^p, \boldsymbol{\sigma}_{n+1}) + \frac{\partial b_p}{\partial \dot{\boldsymbol{\varepsilon}}^p}\left(\boldsymbol{\sigma}_{n+1}, \frac{\boldsymbol{\varepsilon}_{n+1}^p - \boldsymbol{\varepsilon}_n^p}{\Delta t}\right) = 0 \quad (17)$$

158 The values of local fields at time  $t_{n+1}$  ( $\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\varepsilon}_{n+1}^p, \boldsymbol{\sigma}_{n+1}$ ) are unknown, while their values at time  $t_n$   
 159 ( $\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}_n^p, \boldsymbol{\sigma}_n$ ) are assumed to be all known. We introduce here the following incremental bi-potential  $J$ ,  
 160 a scalar-valued function of variables  $\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p$  and  $\boldsymbol{\sigma}$ :

$$J(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) = b_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) + \Delta t b_p\left(\boldsymbol{\sigma}, \frac{\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p}{\Delta t}\right) \quad (18)$$

161 Again, for the sake of abbreviation, the subscripts  $n + 1$  are omitted. Notice that the second relation  
 162 in (17) is the Euler-Lagrange equation of the variational problem for the minimization of incremental  
 163 bi-potential with respect to  $\boldsymbol{\varepsilon}^p$ . This leads to the following condensed incremental bi-potential:

$$\pi_\Delta(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) = \inf_{\boldsymbol{\varepsilon}^p} J(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}, \boldsymbol{\varepsilon}^p) \quad (19)$$

164 After that, the local stress field  $\boldsymbol{\sigma}$  can be derived from this sole bi-potential

$$\boldsymbol{\sigma} = \frac{\partial \pi_\Delta}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) \quad (20)$$

## 165 3. Bi-potential based incremental variational method for homogenization of heterogeneous rocks

166 In this section, a bi-potential theory based incremental variational method (BIV) is developed for  
 167 the estimation of effective elastic-plastic behavior of heterogeneous rocks in the framework of implicit  
 168 standard materials (ISMs) and with the help of the bi-potential theory defined above.

169 *3.1. Representative Volume Element (RVE) and constituents properties*

170 As already shown in Figure 1, the Representative Volume Element (RVE) of rocks at the selected  
 171 length scale (micrometer) is composed of an isotropic elastic-plastic solid matrix in which elastic in-  
 172 clusions (mineral grains) or pores are randomly embedded. The RVE occupies the domain  $\Omega \subset \mathbb{R}^{n_{\text{dim}}}$   
 173 ( $n_{\text{dim}} = 1, 2, 3$ ) with the external boundary  $\Omega \subset \mathbb{R}^{n_{\text{dim}}-1}$ . The solid matrix occupies the sub-domain  
 174  $\Omega^m \subset \mathbb{R}^{n_{\text{dim}}}$ . The elastic property of the matrix is characterized by the elastic stiffness tensor  $\mathbb{C}^m$   
 175 and the plastic behavior is described by a non-associated plastic model with Drucker-Prager yield  
 176 criterion. The  $r^{\text{th}}$  phase of inclusions occupies the sub-domain  $\Omega^{i,r} \subset \mathbb{R}^{n_{\text{dim}}}$ ,  $r = 1, \dots, N$ , and is char-  
 177 acterized by the elastic stiffness tensor  $\mathbb{C}^{i,r}$ . The phase of pores is here treated as a special inclusion  
 178 phase with a vanished elastic stiffness.

179 For the convenience of the subsequent formulation, the total volume of the RVE is denoted as  $V_\Omega$ ,  
 180 the volume of matrix as  $V_{\Omega^m}$ , and the volume occupied by the  $r^{\text{th}}$  inclusion phase as  $V_{\Omega^{i,r}}$ . Accordingly,  
 181 the volume fractions of the constituents are given by:

$$f^m = \frac{V_{\Omega^m}}{V_\Omega}; \quad f^{i,r} = \frac{V_{\Omega^{i,r}}}{V_\Omega}, \quad r = 1, \dots, N; \quad (21)$$

182 Further, the operator  $\langle \cdot \rangle$  denotes a volume average over the whole RVE,  $\langle \cdot \rangle_m$  is a volume average over  
 183 the matrix, and  $\langle \cdot \rangle_{i,r}$  is a volume average over the  $r^{\text{th}}$  inclusion phase. That is

$$\langle \cdot \rangle = \frac{1}{V_\Omega} \int_{V_\Omega} (\cdot) dV_\Omega = f^m \langle \cdot \rangle_m + \sum_{r=1}^N f^{i,r} \langle \cdot \rangle_{i,r} \quad (22)$$

184 with

$$\langle \cdot \rangle_m = \frac{1}{V_{\Omega^m}} \int_{V_{\Omega^m}} (\cdot) dV_{\Omega^m}; \quad \langle \cdot \rangle_{i,r} = \frac{1}{V_{\Omega^{i,r}}} \int_{V_{\Omega^{i,r}}} (\cdot) dV_{\Omega^{i,r}} \quad (23)$$

185 *3.1.1. Incremental bi-potential of the elastic and non-associated Drucker-Prager perfectly plastic*  
 186 *matrix*

187 By assuming that the elastic behaviour is independent of irreversible process, the elastic bi-  
 188 potential  $b_e^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma})$  at any point  $\underline{x} \in \Omega^m$  is written as:

$$b_e^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) : \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + \frac{1}{2} \boldsymbol{\sigma} : \mathbb{S}^m : \boldsymbol{\sigma} \quad (24)$$

189 where the isotropic elastic stiffness tensor is expressed as  $\mathbb{C}^m = 3k^m \mathbb{J} + 2\mu^m \mathbb{K}$ , with  $k^m$  and  $\mu^m$  being  
 190 the bulk modulus and shear modulus of the matrix respectively.  $\mathbb{S}^m = [\mathbb{C}^m]^{-1}$  is the elastic compliance  
 191 tensor.

192 The Drucker-Prager plastic yield function is illustrated in Figure 2 and is written as:

$$\mathcal{F}(\boldsymbol{\sigma}) = \sigma_{eq} + 3\kappa(\sigma_m - c) \leq 0 \quad (25)$$

193 where  $\sigma_{eq} = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$  is the equivalent stress (with  $\mathbf{s} = \boldsymbol{\sigma} : \mathbb{K}$ ), and  $\sigma_m = \frac{1}{3} \boldsymbol{\sigma} : \boldsymbol{\delta}$  the mean stress. The  
 194 parameter  $c$  and  $\kappa$  respectively represent the hydrostatic tensile strength and friction coefficient. It is  
 195 noted that  $\kappa$  is related to the friction angle  $\phi$  as follows:

$$\tan \phi = 3\kappa \quad (26)$$

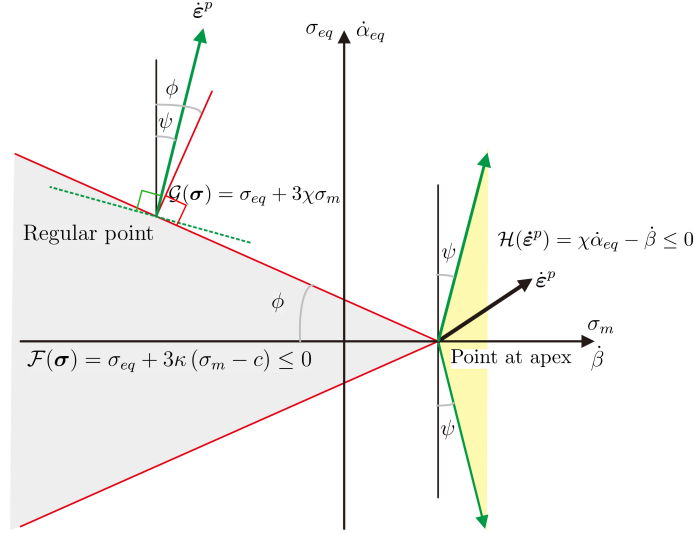


Figure 2: Drucker-Prager yield surface and non-associated plastic flow rule

196 The non-associated plastic flow rule is defined by the following plastic potential:

$$\mathcal{G}(\boldsymbol{\sigma}) = \sigma_{eq} + 3\chi\sigma_m \quad (27)$$

197 where  $\chi$  denotes the plastic dilatancy coefficient, which depends on the dilatancy angle  $\psi$ :

$$\tan \psi = 3\chi \quad (28)$$

198 Further, for any stress state located on the regular part of the yield surface, it is assumed that the  
 199 plastic dilatancy coefficient  $\chi$  is equal or less than the friction coefficient, i.e.,  $\chi \leq \kappa$  (Hjiaj et al.,  
 200 2003). The corresponding rate form of plastic strain  $\boldsymbol{\varepsilon}^p$  is defined by the non-associated flow rule:

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}^p \frac{\partial \mathcal{G}}{\partial \boldsymbol{\sigma}} = \dot{\gamma}^p \left( \frac{3}{2} \frac{\mathbf{s}}{\sigma_{eq}} + \chi \boldsymbol{\delta} \right) \quad (29)$$

201 where  $\dot{\gamma}^p$  is a non-negative internal variable acting as the plastic multiplier. For convenience, the  
 202 plastic strain tensor is decomposed into a spherical part and a deviatoric part:

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\alpha} + \boldsymbol{\beta}, \quad \boldsymbol{\alpha} = \boldsymbol{\varepsilon}^p : \mathbb{K}, \quad \boldsymbol{\beta} = \boldsymbol{\varepsilon}^p : \mathbb{J} = \frac{1}{3} \text{tr} \boldsymbol{\varepsilon}^p \boldsymbol{\delta} = \beta \boldsymbol{\delta} \quad (30)$$

203 One thus obtains:

$$\dot{\gamma}^p = \sqrt{\frac{2}{3}} \dot{\boldsymbol{\alpha}} : \dot{\boldsymbol{\alpha}} = \dot{\alpha}_{eq}, \quad \dot{\boldsymbol{\alpha}} = \mathbb{K} : \dot{\boldsymbol{\varepsilon}}^p, \quad \dot{\beta} = \frac{1}{3} \text{tr} \dot{\boldsymbol{\varepsilon}}^p = \chi \dot{\alpha}_{eq} \quad (31)$$

204 Again for convenience we introduce

$$\mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) = \chi \dot{\alpha}_{eq} - \dot{\beta} \quad (32)$$

205 Considering now a stress state at the apex point ( $\sigma_{eq} = 0, \sigma_m = c$ ) of the Drucker-Prager yield  
 206 surface,  $\mathcal{F}(\boldsymbol{\sigma})$  is not differentiable, and the plastic strain rate tensor is not unique. In this case, one  
 207 gets  $\mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) \leq 0$  (see Figure 2). It is obviously noticed from Eq. (31) that  $\mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) = 0$  for the points  
 208 on the regular part of the yield surface. Therefore, the plastic flow rule (29) is completed by the  
 209 admissibility condition of the plastic strain rate for all the cases

$$\mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) \leq 0 \quad (33)$$

210 According to Hjiatj et al. (2003), the plastic bi-potential for the non-associated Drucker-Prager  
 211 plastic flow without strain hardening takes the following form:

$$b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) = \begin{cases} 3c\dot{\beta} + 3(\chi - \kappa)(\sigma_m - c)\dot{\alpha}_{eq} & \text{if } \mathcal{F}(\boldsymbol{\sigma}) \leq 0 \text{ and } \mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) \leq 0 \\ +\infty & \text{otherwise} \end{cases} \quad (34)$$

212 The proof that the function (34) is a bi-potential has been given in Hjiatj et al. (2003). It is noted that  
 213 the above express is defined for the regular stress points. In this case, the function (34) can be further  
 214 rewritten as

$$b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\varepsilon}}^p) = b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\alpha}}) = \begin{cases} \underbrace{[3\sigma_m(\chi - \kappa) + 3c\kappa]}_{\sigma_y} \dot{\alpha}_{eq} = \sigma_y \dot{\alpha}_{eq} & \text{if } \mathcal{F}(\boldsymbol{\sigma}) \leq 0 \text{ and } \mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) = 0 \\ +\infty & \text{otherwise} \end{cases} \quad (35)$$

215 *Remark 1.* The second part of the first line in the right hand side of Eq. (35) contains a mixed term of  
 216 stress and plastic strain rate. When  $\chi = \kappa$ , the mixed term disappears and the bi-potential  $b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\alpha}})$   
 217 reduces to the plastic dissipation potential  $\varphi^m(\dot{\boldsymbol{\alpha}})$  for GSMs.

$$b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\alpha}}) = \varphi^m(\dot{\boldsymbol{\alpha}}) = \begin{cases} 3c\kappa \dot{\alpha}_{eq} & \text{if } f(\boldsymbol{\sigma}) \leq 0 \text{ and } \mathcal{H}(\dot{\boldsymbol{\varepsilon}}^p) = 0 \\ +\infty & \text{otherwise} \end{cases} \quad (36)$$

218 Inserting the elastic bi-potential (24) and plastic bi-potential(35) into Eq.(19), one finally obtains  
 219 the local incremental bi-potential  $\pi_\Delta^m$  of the elastic non-associated perfectly plastic matrix:

$$\pi_\Delta^m(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) = \inf_{\boldsymbol{\varepsilon}^p} J^m(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}, \boldsymbol{\varepsilon}^p) = \inf_{\boldsymbol{\varepsilon}^p} \left( b_e^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) + \Delta t b_p^m \left( \boldsymbol{\sigma}, \frac{\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p}{\Delta t} \right) \right) \quad (37)$$

220 *3.1.2. Behavior of elastic inclusion*

221 At any point inside the  $r^{\text{th}}$  linear elastic inclusion phase, i.e.,  $\underline{x} \in \Omega^{i,r}$ , the elastic bi-potential  $b_e^{i,r}$   
 222 is the convex function of local strain field  $\boldsymbol{\varepsilon}$  and stress field  $\boldsymbol{\sigma}$ . Accordingly, the local incremental  
 223 bi-potential  $\pi_\Delta^{i,r}$  of the  $r^{\text{th}}$  elastic inclusion phase is expressed as:

$$\pi_\Delta^{i,r} = b_e^{i,r}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbb{C}^{i,r} : \boldsymbol{\varepsilon} + \frac{1}{2} \boldsymbol{\sigma} : \mathbb{S}^{i,r} : \boldsymbol{\sigma} \quad (38)$$

224 *3.2. Effective behavior of heterogeneous rocks*

225 We consider that the RVE of heterogeneous rocks is subjected to a macroscopic strain  $\bar{\boldsymbol{\varepsilon}}(t)$ , and  
 226 for definiteness, to the periodic kinematic boundary conditions on its boundary  $\partial\Omega$  at time step  $t_{n+1}$ .  
 227 Due to the time-discretization scheme adopted, the local problem to be solved is formulated as fol-  
 228 lows:

$$\left\{ \begin{array}{l} \text{div } \boldsymbol{\sigma}_{n+1} = 0 \\ \boldsymbol{\sigma}_{n+1} = \frac{\partial \pi_\Delta}{\partial \boldsymbol{\varepsilon}_{n+1}}(\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\sigma}_{n+1}) \\ \langle \boldsymbol{\varepsilon}(t) \rangle = \bar{\boldsymbol{\varepsilon}}(t) + BC \text{ on } \partial\Omega \end{array} \right\} \text{ for } (\underline{x}, t) \in \Omega \times [0, T] \quad (39)$$

229 The condensed incremental bi-potential  $\pi_\Delta(\underline{x}, \boldsymbol{\varepsilon}, \boldsymbol{\sigma})$  in the RVE is here defined as:

$$\pi_\Delta = \begin{cases} \pi_\Delta^m & \text{if } \underline{x} \in \Omega^m \\ \pi_\Delta^{i,r} & \text{if } \underline{x} \in \Omega^{i,r} \end{cases} \quad (40)$$

230 Finally, the macroscopic stress  $\bar{\boldsymbol{\sigma}}$  can be derived from the effective incremental bi-potential of the  
 231 RVE:

$$\bar{\boldsymbol{\sigma}}_{n+1} = \frac{\partial \Pi_\Delta}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}_{n+1}, \bar{\boldsymbol{\sigma}}_{n+1}) \quad (41)$$

232 The effective incremental bi-potential  $\Pi_\Delta$  is here determined by using the variational principle:

$$\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}_{n+1}, \bar{\boldsymbol{\sigma}}_{n+1}) = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}_{n+1}} \langle \pi_\Delta \rangle = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}_{n+1}} \left[ f^m \left\langle \inf_{\boldsymbol{\varepsilon}^p} J^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \right\rangle_m + \sum_{r=1}^N f^{i,r} \left\langle b_e^{i,r}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) \right\rangle_{i,r} \right] \quad (42)$$

233 The effective incremental bi-potential of the RVE is not only related to the macroscopic strain  $\bar{\boldsymbol{\varepsilon}}$ ,  
 234 but also to the average value of local stress field  $\boldsymbol{\sigma}$  on the RVE. With this single effective bi-potential  
 235 in hand, according to Eq. (41), the macroscopic stress is the conjugated force associated with the  
 236 macroscopic strain, which is consistent with the classical thermodynamic framework. Moreover, the  
 237 macroscopic stress defined here also coincides with the volumetric average of the local stress field

238 over the RVE. Accordingly, the problem of computing the overall response of the heterogeneous  
 239 materials comes to solving the variational problem (42) at each time step, which itself involves a local  
 240 optimization problem (37) with respect to the internal variables (plastic strain)  $\boldsymbol{\varepsilon}^p$  at every position  
 241  $\underline{x} \in \Omega^m$ . Instead of searching a computationally-costly full-field numerical solution, an approximated  
 242 solutions is found in Section 4 by using the variational procedure initially proposed in [Lahellec and](#)  
 243 [Suquet \(2007b\)](#) for GSMs.

#### 244 4. Optimization of the effective incremental bi-potential

245 The main steps for the estimation of the effective incremental bi-potential through a variational  
 246 procedure are presented in this section.

##### 247 4.1. Approximation of local incremental bi-potential of the elastic perfectly-plastic matrix

248 The first step is to approximate the local incremental bi-potential  $J^m$  given in (37). It is noticed that  
 249 the elastic bi-potential given in (24) includes the plastic volumetric strain  $\boldsymbol{\beta}$ . For ease of calculation  
 250 and taking advantage of the main results obtained in [Lahellec and Suquet \(2007b\)](#), the elastic bi-  
 251 potential (24) is approximated and the plastic bi-potential (35) is linearized as follows.

- 252 • Approximation of local elastic bi-potential  $b_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma})$  (see detailed process in [Appendix A](#))

$$b_e^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \simeq b_e^{app}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{\sigma} : \mathbb{S}^m : \boldsymbol{\sigma} + \frac{1}{2} \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi \boldsymbol{\delta}}} \right) : \mathbb{C}^m : \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi \boldsymbol{\delta}}} \right) \quad (43)$$

- 253 • For the plastic bi-potential  $b^p(\boldsymbol{\sigma}, \dot{\boldsymbol{\alpha}})$  here we use the same variational linearization procedure  
 254 and take the same quadratic form as those used in [Lahellec and Suquet \(2007b\)](#) and [Boudet et al.](#)  
 255 (2016), i.e.  $\frac{\eta_0}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n)$ . In this expression, the scalar variable  $\eta_0$  and second-order  
 256 tensor  $\tilde{\boldsymbol{\alpha}}_n$  are uniform in the elastic-plastic matrix.

257 With the above simplifications in hand, the local incremental bi-potential  $J^m$  in (37) can be ap-  
 258 proximated as

$$\left\{ \begin{array}{l} J^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \simeq J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \\ J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi \boldsymbol{\delta}}} \right) : \mathbb{C}^m : \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi \boldsymbol{\delta}}} \right) + \frac{\eta_0}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \\ \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{\sigma} : \mathbb{S}^m : \boldsymbol{\sigma} + \sigma_y (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n)_{eq} - \frac{\eta_0}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \end{array} \right. \quad (44)$$

259 where  $J_0^m$  is the linearized local incremental potential in the matrix phase.

260 4.2. Estimation of the effective incremental bi-potential  $\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}_m)$

261 The effective incremental bi-potential of the RVE is determined by calculating the volumetric  
262 average of the two terms of the local incremental bi-potential given in Eq. (44):

$$\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}) = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \left[ f^m \left\langle \inf_{\boldsymbol{\alpha}} (J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha})) \right\rangle_m + \sum_{r=1}^N f^{i,r} \left\langle b_e^{i,r}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) \right\rangle_{i,r} \right] \quad (45)$$

263 The secant function  $\eta_{sct}(\dot{\boldsymbol{\alpha}}_{eq}, \boldsymbol{\sigma})$  of the matrix phase is defined as (Lahellec and Suquet, 2007b):

$$\eta_{sct}(\dot{\boldsymbol{\alpha}}_{eq}, \boldsymbol{\sigma}) = \frac{1}{3\dot{\boldsymbol{\alpha}}_{eq}} \frac{\partial b_p^m}{\partial \dot{\boldsymbol{\alpha}}_{eq}}(\boldsymbol{\sigma}, \boldsymbol{\alpha}) = \frac{\sigma_y}{3\dot{\boldsymbol{\alpha}}_{eq}} \quad (46)$$

264 and Eq. (45) satisfies

$$\Pi_\Delta^m(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}) \leq \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \left\{ f^m \left[ \left\langle \inf_{\boldsymbol{\alpha}} J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) \right\rangle_m + \left\langle \sup_{\boldsymbol{\alpha}} \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \right\rangle_m \right] + \sum_{r=1}^N f^{i,r} \left\langle b_e^{i,r}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) \right\rangle_{i,r} \right\} \quad (47)$$

265 Note that the local optimization problem in Eq. (47) is solved with respect to the internal variable  $\boldsymbol{\alpha}$   
266 only instead of the set of variables  $(\boldsymbol{\alpha}, \boldsymbol{\beta})$  as defined in Eq.(37) at every point  $\underline{x} \in \Omega_m$ . This largely de-  
267 duces the complexity of the local optimization problem. The estimate (47) of the effective bi-potential  
268  $\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}})$  with the non-associated perfectly plastic matrix has the similar form as that pertained to  
269 nonlinear viscoelastic composites without hardening studied in Lahellec and Suquet (2007b).

270 According to previous studies (Castañeda and Willis, 1999, Castañeda, 2002, Lahellec and Suquet,  
271 2007b), sharper estimates of  $\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}})$  can be obtained by requiring only the stationarity of  $\Delta J^m$   
272 instead of its supremum with respect to  $\boldsymbol{\alpha}$ . Therefore, one gets:

$$\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}) \simeq \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \left\{ f^m \left[ \left\langle \inf_{\boldsymbol{\alpha}} J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) \right\rangle_m + \left\langle \text{stat} \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \right\rangle_m \right] + \sum_{r=1}^N f^{i,r} \left\langle b_e^{i,r}(\boldsymbol{\varepsilon}, \boldsymbol{\sigma}) \right\rangle_{i,r} \right\} \quad (48)$$

273 It is worth noticing that the difference function in the increment potential  $\Delta J^m$  is generally non-  
274 quadratic. In order to determine the stationarity of  $\Delta J^m$  with respect to  $\boldsymbol{\alpha}$ , we rewrite the plastic  
275 bi-potential in the following form:

$$b_p^m(\boldsymbol{\sigma}, \dot{\boldsymbol{\alpha}}) = Y(\boldsymbol{\sigma}, \frac{(\boldsymbol{\alpha} - \boldsymbol{\alpha}_n)_{eq}^2}{\Delta t^2}) \quad (49)$$

276 The concavity of  $Y$  ensures that  $\langle Y(\boldsymbol{\sigma}, \boldsymbol{a}) \rangle_m \leq Y(\langle \boldsymbol{\sigma} \rangle_m, \langle \boldsymbol{a} \rangle_m)$  for any field  $\boldsymbol{a}(\underline{x})$ . One then gets the  
277 following order relation:

$$\langle \Delta J^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \rangle_m \leq \langle \Delta \tilde{J}^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \rangle_m = \frac{1}{2} \langle \boldsymbol{\sigma} \rangle_m : \mathbb{S}^m : \langle \boldsymbol{\sigma} \rangle_m + \Delta t Y \left( \left\langle \boldsymbol{\sigma}, \frac{(\boldsymbol{\alpha} - \boldsymbol{\alpha}_n)_{eq}^2}{\Delta t^2} \right\rangle_m \right) - \left\langle \frac{\eta_0}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \right\rangle_m \quad (50)$$

278 The stationarity of  $\langle \Delta \tilde{J}^m(\boldsymbol{\sigma}, \boldsymbol{\alpha}) \rangle_m$  with respect to  $\boldsymbol{\alpha}$  yields

$$2\eta_p \frac{(\boldsymbol{\alpha} - \boldsymbol{\alpha}_n)}{\Delta t} = 2\eta_0 \frac{(\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n)}{\Delta t} \quad (51)$$

279 The coefficient  $\eta_p$  is the secant viscosity associated with the plastic material without hardening and  
280 given by:

$$\eta_p = \eta_{sct}(\bar{\dot{\boldsymbol{\alpha}}}, \langle \boldsymbol{\sigma} \rangle_m) = \frac{\langle \sigma_y \rangle_m}{3\bar{\dot{\boldsymbol{\alpha}}}}, \quad \text{with } \bar{\dot{\boldsymbol{\alpha}}} = \sqrt{\frac{2}{3} \langle \dot{\boldsymbol{\alpha}} : \dot{\boldsymbol{\alpha}} \rangle_m} \quad (52)$$

281 It is noticed that (51) can be rewritten in the following form:

$$\boldsymbol{\alpha} = \frac{\boldsymbol{\alpha}_n - \theta \tilde{\boldsymbol{\alpha}}_n}{1 - \theta}, \quad \text{with } \theta = \frac{\eta_0}{\eta_p} \quad (53)$$

282 With this relation, the last term in (48) can be evaluated and  $\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}})$  can be further estimated as  
283 follows:

$$\Pi_\Delta(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}) \simeq \Pi_0(\bar{\boldsymbol{\varepsilon}}) + \Delta \Pi^m(\bar{\boldsymbol{\sigma}}) \quad (54)$$

with

$$\Pi_0(\bar{\boldsymbol{\varepsilon}}) = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \left[ f^m \left\langle \inf_{\boldsymbol{\alpha}} J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) \right\rangle_m + \frac{1}{2} \sum_{r=1}^N f^{i,r} \langle \boldsymbol{\varepsilon} \rangle_{i,r} : \mathbb{C}^{i,r} : \langle \boldsymbol{\varepsilon} \rangle_{i,r} \right] \quad (55a)$$

$$\Delta \Pi^m(\bar{\boldsymbol{\sigma}}) = f^m \left( \frac{1}{2} \langle \boldsymbol{\sigma} \rangle_m : \mathbb{S}^m : \langle \boldsymbol{\sigma} \rangle_m + \left\langle \frac{\eta_p \theta}{\Delta t (\theta - 1)} (\boldsymbol{\alpha}_n - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha}_n - \tilde{\boldsymbol{\alpha}}_n) \right\rangle_m \right) + \frac{1}{2} \sum_{r=1}^N f^{i,r} \langle \boldsymbol{\sigma} \rangle_{i,r} : \mathbb{S}^{i,r} : \langle \boldsymbol{\sigma} \rangle_{i,r} \quad (55b)$$

284 By using the stationarity condition of (54) over  $\tilde{\boldsymbol{\alpha}}_n$  and  $\theta$ , one gets:

$$\theta = 1 \pm \sqrt{\frac{\langle (\boldsymbol{\alpha}_n - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha}_n - \tilde{\boldsymbol{\alpha}}_n) \rangle_m}{\langle (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) : (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \rangle_m}} \quad (56)$$

$$\tilde{\boldsymbol{\alpha}}_n = \frac{\langle \boldsymbol{\alpha}_n \rangle_m + (\theta - 1) \langle \boldsymbol{\alpha} \rangle_m}{\theta} \quad (57)$$

285 It is noticed that in the aforementioned calculations, the sign '-' is adopted in Eq. (56), which corre-  
286 sponds to solving the problem (47) with an infimum and therefore to a rigorous lower bound for the  
287 effective bi-potential  $\Pi_\Delta$ .

288 With the help of minimization of  $J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$  with respect to  $\boldsymbol{\alpha}$ , one finally obtains (the detailed  
289 calculation is given in Appendix B):

$$\boldsymbol{\alpha} = \left( \mathbb{C}^m + \frac{2\theta\eta}{\Delta t} \mathbb{K} \right)^{-1} : \left[ \mathbb{K} : \mathbb{C}^m : \boldsymbol{\varepsilon} + \frac{2\theta\eta}{\Delta t} \tilde{\boldsymbol{\alpha}}_n \right] = d \mathbb{K} : \boldsymbol{\varepsilon} + e \tilde{\boldsymbol{\alpha}}_n \quad (58a)$$

290 where  $d = \frac{\mu}{\frac{\eta_0}{\Delta t} + \mu}$ ,  $e = \frac{\frac{\eta_0}{\Delta t}}{\frac{\eta_0}{\Delta t} + \mu}$ .  $\eta$  denotes the uniform total secant viscosity taken at  $\bar{\dot{\boldsymbol{\alpha}}}$  of the non-

291 associated plastic matrix without hardening:

$$\eta(\bar{\dot{\boldsymbol{\alpha}}}, \langle \boldsymbol{\sigma} \rangle_m) = -\frac{\kappa(\langle \sigma_m \rangle_m - c)}{\bar{\dot{\boldsymbol{\alpha}}}} \quad (59)$$



### 292 4.3. Estimation of the effective potential $\Pi_0(\bar{\boldsymbol{\varepsilon}})$ of homogenized material

293 The last step of formulation is the estimation of the effective potential  $\Pi_0(\bar{\boldsymbol{\varepsilon}})$  of the homogenized  
 294 equivalent material (HEM) in order to estimate the macroscopic elastic-plastic behavior of the hetero-  
 295 geneous rocks. This is based on the choice of a thermoelastic linear comparison composite (LCC).  
 296 Substituting the result found in (58a) for the expression of  $J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$  in (44) and making use of Eq.  
 297 (53), one defines the local increment potential  $\pi_0^m(\boldsymbol{\varepsilon})$  of the LCC as follows:

$$\pi_0^m(\boldsymbol{\varepsilon}) = \inf_{\boldsymbol{\alpha}} J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbb{C}_0^m : \boldsymbol{\varepsilon} + \boldsymbol{\rho}_0^m : \boldsymbol{\varepsilon} + \zeta_0^m \quad (60)$$

298 The tensors  $\mathbb{C}_0^m$  and  $\boldsymbol{\rho}_0^m$  as well as the scalar coefficient  $\zeta_0^m$  are all uniform in the matrix phase and  
 299 given by:

$$\left\{ \begin{array}{l} \mathbb{C}_0^m = 3k^m \mathbb{J} + 2\mu_0^m \mathbb{K}, \quad \text{with } \mu_0^m = (1-d)^2 \mu^m + \frac{\theta \eta_p}{\Delta t} d^2 \\ \boldsymbol{\rho}_0^m = 2 \left[ \frac{\theta \eta_p}{\Delta t} d(e-1) - \mu^m(1-d) \right] \tilde{\boldsymbol{\alpha}}_n - 3k^m \left( \langle \boldsymbol{\beta}_n \rangle_m + \overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi} \boldsymbol{\delta} \right) \\ \zeta_0^m = \left[ e^2 \mu^m + \frac{\theta \eta_p}{\Delta t} (e-1)^2 \right] \tilde{\boldsymbol{\alpha}}_n : \tilde{\boldsymbol{\alpha}}_n + \frac{9}{2} k^m \left( \langle \boldsymbol{\beta}_n \rangle_m + \overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n \chi} \right)^2 \end{array} \right. \quad (61)$$

300 The quantities  $\theta$ ,  $\tilde{\boldsymbol{\alpha}}_n$  and  $\eta$  are defined in Eqs. (56), (57) and (59), respectively. Further, the effective  
 301 potential  $\Pi_0(\bar{\boldsymbol{\varepsilon}})$  defined in Eq. (55a) can be written as

$$\Pi_0(\bar{\boldsymbol{\varepsilon}}) = \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\rho}} : \bar{\boldsymbol{\varepsilon}} + \bar{\zeta} \quad (62)$$

302 The effective tensors  $\bar{\mathbb{C}}$  and  $\bar{\boldsymbol{\rho}}$  as well as the scalar variable  $\bar{\zeta}$  are expressed in Appendix C.

303 By using the expression of  $\Pi_0(\bar{\boldsymbol{\varepsilon}})$  (Eq. (62)) in (55a), the macroscopic stress tensor  $\bar{\boldsymbol{\sigma}}$  of the HEM  
 304 as that defined in Eq. (41) can be approximated by the following differentiation procedure:

$$\bar{\boldsymbol{\sigma}} = \frac{\partial \Pi_\Delta}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\sigma}}) = \frac{d\Pi_0}{d\bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}) = f^m \langle \boldsymbol{\sigma} \rangle_m + \sum_{r=1}^N f^{i,r} \langle \boldsymbol{\sigma} \rangle_{i,r} \quad (63)$$

with

$$\langle \boldsymbol{\sigma} \rangle_m = \mathbb{C}_0^m : \langle \boldsymbol{\varepsilon} \rangle_m + \boldsymbol{\rho}_0 \quad (64a)$$

$$\langle \boldsymbol{\sigma} \rangle_{i,r} = \mathbb{C}^{i,r} : \langle \boldsymbol{\varepsilon} \rangle_{i,r} \quad (64b)$$

## 305 5. Fluctuations of local fields and computational aspects

### 306 5.1. Fluctuations of local fields in matrix

307 In order to assess the accuracy of the BIV model, not only the macroscopic responses of the  
 308 HEM but also the representative fluctuations of local fields should be investigated. In this study, we

309 shall evaluate the fluctuations of local stress and plastic strain fields in the matrix. The fluctuations  
 310 of interest contain the first- and second-order moments of the these fields. Following [Idiart and](#)  
 311 [Castañeda \(2007\)](#) the quadratic fluctuation of the local stress in the matrix is defined as

$$\mathbb{F}_{\sigma}^m \equiv \langle \sigma - \langle \sigma \rangle_m \rangle_m \otimes \langle \sigma - \langle \sigma \rangle_m \rangle_m = \langle \sigma \otimes \sigma \rangle_m - \langle \sigma \rangle_m \otimes \langle \sigma \rangle_m \quad (65)$$

312 where  $\langle \sigma \rangle_m$  and  $\langle \sigma \otimes \sigma \rangle_m$  represent the first and second-order moment of local stress field over the  
 313 matrix.  $\langle \sigma \rangle_m$  can be obtained from the relation (64a). However it is generally difficult to calculate  
 314  $\langle \sigma \otimes \sigma \rangle_m$ . In order to amend this issue, here we adopt the following expression proposed in ([Agoras](#)  
 315 [et al., 2016](#)):

$$\sqrt{\mathbb{F}_{\sigma}^m} :: \mathbb{K} = \sqrt{\langle s : s \rangle_m - \langle s \rangle_m : \langle s \rangle_m} = \sqrt{\frac{2}{3} \left( \bar{\bar{\sigma}}^2 - (\bar{\sigma}_{eq}^m)^2 \right)} \quad (66)$$

316 with  $\bar{\sigma}_{eq}^m = \sqrt{\frac{3}{2} \langle s \rangle_m : \langle s \rangle_m}$  and  $\bar{\bar{\sigma}} = \sqrt{\frac{3}{2} \langle s : s \rangle_m}$  for the evaluation of  $\langle s \rangle_m$  and  $\langle s : s \rangle_m$ . Together with  
 317 Eq. (B.9), one further obtains

$$\bar{\bar{\sigma}} = 3\eta\bar{\bar{\alpha}} \quad (67)$$

318 The calculation of the denominator  $\bar{\bar{\alpha}}$  is given in Section 5.3. One can notice that it is easy to obtain  
 319 the fluctuation of local stress field (66) with the help of Eqs. (64a) and (67).

320 Similarly, the fluctuation of the local plastic strain field in the matrix is defined as:

$$\mathbb{F}_{\epsilon^p}^m \equiv \langle \epsilon^p - \langle \epsilon^p \rangle_m \rangle_m \otimes \langle \epsilon^p - \langle \epsilon^p \rangle_m \rangle_m = \langle \epsilon^p \otimes \epsilon^p \rangle_m - \langle \epsilon^p \rangle_m \otimes \langle \epsilon^p \rangle_m \quad (68)$$

321 where  $\langle \epsilon^p \rangle_m$  and  $\langle \epsilon^p \otimes \epsilon^p \rangle_m$  represent the first and second-order moments of local plastic strain field  
 322 over the matrix. For the ease of calculation, we provide the result for the standard derivation of the  
 323 plastic strain filed in the matrix phase, that is:

$$\sqrt{\mathbb{F}_{\epsilon^p}^m} :: \mathbb{K} = \sqrt{\langle \alpha : \alpha \rangle_m - \langle \alpha \rangle_m : \langle \alpha \rangle_m} = \sqrt{\frac{3}{2} \left( \bar{\bar{\alpha}}^2 - (\bar{\alpha}_{eq}^m)^2 \right)} \quad (69)$$

324 with  $\bar{\alpha}_{eq}^m = \sqrt{\frac{2}{3} \langle \alpha \rangle_m : \langle \alpha \rangle_m}$  and  $\bar{\bar{\alpha}} = \sqrt{\frac{2}{3} \langle \alpha : \alpha \rangle_m}$ , being the first- and second-order moment of  $\alpha$ .

## 325 5.2. Computation of the first and second-order moment of $\alpha$

326 The calculation of  $\theta$ ,  $\tilde{\alpha}_n$  and  $\sqrt{\mathbb{F}_{\epsilon^p}^m} :: \mathbb{K}$  from Eqs.(56), (57) and (69) needs the determination of  
 327 the first- and second-order moment of  $\alpha$  in the plastic matrix. The first moment is given by:

$$\langle \alpha \rangle_m = \langle d\mathbb{K} : \epsilon + e\tilde{\alpha}_n \rangle_m \quad (70)$$

328 Since the quantities  $d$ ,  $e$  and  $\tilde{\alpha}_n$  are uniform in the matrix phase, one thus obtains

$$\langle \alpha \rangle_m = d\mathbb{K} : \langle \epsilon \rangle_m + e : \tilde{\alpha}_n \quad (71)$$

329 Similarly, the second-order moment of  $\alpha$  is calculated by:

$$\langle \alpha : \alpha \rangle_m = d^2 \mathbb{K} :: \langle \varepsilon \otimes \varepsilon \rangle_m + 2de\tilde{\alpha}_n : \langle \varepsilon \rangle_m + e^2\tilde{\alpha}_n : \tilde{\alpha}_n \quad (72)$$

330 The first and second terms at the right hand side of Eq. (72) are related to the second- and first-order  
331 moments of  $\varepsilon$  in the matrix phase and can be obtained from Eqs.(C.6) and (C.3), respectively.

### 332 5.3. Computation of the second-order moment of $\dot{\alpha}$

333 To calculate  $\eta$  from Eq. (59), the denominator  $\overline{\dot{\alpha}}$  related to the second-order moment of  $\dot{\alpha}$  should  
334 be first determined by:

$$\overline{\dot{\alpha}} = \sqrt{\frac{2}{3} \langle \dot{\alpha} : \dot{\alpha} \rangle_m} = \frac{1}{\Delta t} \sqrt{\frac{2}{3} \langle (\alpha - \alpha_n) : (\alpha - \alpha_n) \rangle_m} \quad (73)$$

335 It is noticed that it is generally difficult to calculate  $\langle (\alpha - \alpha_n) : (\alpha - \alpha_n) \rangle_m$  due to the inaccessibility  
336 of the term  $\langle \alpha : \alpha_n \rangle_m$ . However, thanks to Eq. (57),  $\overline{\dot{\alpha}}$  can be alternatively calculated by the following  
337 relation when  $\theta \neq 1$ :

$$\begin{aligned} \overline{\dot{\alpha}} &= \left[ \frac{\theta}{\Delta t (1 - \theta)} \right] \sqrt{\frac{2}{3} \langle (\alpha_n - \tilde{\alpha}_n) : (\alpha_n - \tilde{\alpha}_n) \rangle_m} \\ &= \left[ \frac{\theta}{\Delta t (1 - \theta)} \right] \sqrt{\frac{2}{3} (\langle \alpha_n : \alpha_n \rangle_m - 2 \langle \alpha_n \rangle_m : \tilde{\alpha}_n + \tilde{\alpha}_n : \tilde{\alpha}_n)} \end{aligned} \quad (74)$$

338 where the first- and second-order moments of  $\alpha$  are already determined from (71) and (72) respec-  
339 tively.

## 340 6. Implementation and numerical assessment of the BIV model

### 341 6.1. Local implementation algorithm of BIV model

342 The numerical implantation algorithm of the proposed BIV model is now presented. This al-  
343 gorithm is developed as a user-defined subroutine for the determination of mechanical behavior of  
344 a macroscopic material point in a standard computation code. The material point is subjected to a  
345 macroscopic strain increment  $\Delta \bar{\varepsilon}$  ( $\Delta \bar{\varepsilon} = \dot{\bar{\varepsilon}} \Delta t$ ) such that  $\bar{\varepsilon}_{n+1} = \bar{\varepsilon}_n + \Delta \bar{\varepsilon}$  at  $t_{n+1}$ . The numerical algo-  
346 rithm is here used to calculate the macroscopic stress increment using the proposed BIV model. The  
347 flowchart of the computational procedure is summarized in Algorithm 1:

---

**Algorithm 1:** Flowchart of the local implementation algorithm of BIV

---

**Input:**  $\dot{\bar{\boldsymbol{\varepsilon}}}, \Delta t, \bar{\boldsymbol{\sigma}}_n, \bar{\boldsymbol{\varepsilon}}_n, \langle \boldsymbol{\alpha}_n \rangle_m, \langle \boldsymbol{\beta}_n \rangle_m, \langle \boldsymbol{\alpha}_n : \boldsymbol{\alpha}_n \rangle_m, \theta_n, \eta_n$ **Output:**  $\bar{\boldsymbol{\sigma}}_{n+1}, \bar{\boldsymbol{\varepsilon}}_{n+1}, \langle \boldsymbol{\alpha}_{n+1} \rangle_m, \langle \boldsymbol{\beta}_{n+1} \rangle_m, \langle \boldsymbol{\alpha}_{n+1} : \boldsymbol{\alpha}_{n+1} \rangle_m, \theta_{n+1}, \eta_{n+1}$ 

- 1  $\bar{\boldsymbol{\varepsilon}}_{n+1} = \bar{\boldsymbol{\varepsilon}}_n + \dot{\bar{\boldsymbol{\varepsilon}}}\Delta t,$
- 2 Initialize  $\eta_{n+1} = \eta_n, \theta_{n+1} = \theta_n$
- 3 Calculate  $\mathbb{A}_{n+1}^m, \mathbb{A}_{n+1}^{i,r}, \mathbf{a}_{n+1}^m, \mathbf{a}_{n+1}^{i,r}, \mathbb{C}_{0,n+1}^m, \boldsymbol{\rho}_{0n+1}^m,$
- 4 Calculate first order moment of strain field  $\langle \boldsymbol{\varepsilon}_{n+1} \rangle_m^{trial} = \mathbb{A}_{n+1}^m : \bar{\boldsymbol{\varepsilon}} + \mathbf{a}_{n+1}^m,$   
 $\langle \boldsymbol{\varepsilon}_{n+1} \rangle_{i,r}^{trial} = \mathbb{A}_{n+1}^{i,r} : \bar{\boldsymbol{\varepsilon}} + \mathbf{a}_{n+1}^{i,r},$
- 5 Elastic prediction:  $\langle \boldsymbol{\sigma}_{n+1} \rangle_m^{trial} = \mathbb{C}^m : (\langle \boldsymbol{\varepsilon}_{n+1} \rangle_m^{trial} - \langle \boldsymbol{\alpha}_n \rangle_m - \langle \boldsymbol{\beta}_n \rangle_m)$
- 6 **if**  $f(\langle \boldsymbol{\sigma}_{n+1} \rangle_m^{trial}) < 0$  **then**
- 7      $\langle \boldsymbol{\varepsilon}_{n+1} \rangle_m = \langle \boldsymbol{\varepsilon}_{n+1} \rangle_m^{trial}; \langle \boldsymbol{\varepsilon}_{n+1} \rangle_{i,r} = \langle \boldsymbol{\varepsilon}_{n+1} \rangle_{i,r}^{trial} \quad \langle \boldsymbol{\alpha}_{n+1} \rangle_m = \mathbf{0}; \langle \boldsymbol{\beta}_{n+1} \rangle_m =$   
       $\mathbf{0}; \langle \boldsymbol{\alpha}_{n+1} : \boldsymbol{\alpha}_{n+1} \rangle_m = 0$
- 8 **else**
- 9     (For clarity, the subscript n+1 will be omitted in the *for* loop)
- 10    **for**  $j = 1 \dots m_{iter},$  **do**
- 11     Calculate  $\mathbb{C}_{0,j}^m, \boldsymbol{\rho}_{0,j}^m, \zeta_{0,j}^m$  and  $\bar{\mathbb{C}}_j$  with Eqs. (61) and (C.2a)
- 12     Calculate  $\mathbb{A}_j^m, \mathbb{A}_j^{i,r}, \mathbf{a}_j^m, \mathbf{a}_j^{i,r}$  (with Eq.(C.7) for two-phases composite).
- 13     Calculate first moment of strain field  $\langle \boldsymbol{\varepsilon} \rangle_{m,j} = \mathbb{A}_j^m : \bar{\boldsymbol{\varepsilon}} + \mathbf{a}_j^m$  and  
       $\langle \boldsymbol{\varepsilon} \rangle_{i,r,j} = \mathbb{A}_j^{i,r} : \bar{\boldsymbol{\varepsilon}} + \mathbf{a}_j^{i,r}$  with Eqs.(C.3) and (C.4);
- 14     Calculate  $\langle \boldsymbol{\sigma} \rangle_{m,j}$  and  $\langle \boldsymbol{\sigma} \rangle_{i,r,j}$  by using Eq.(64);
- 15     Calculate effective internal variable  $\tilde{\boldsymbol{\alpha}}_{n,j}$  and  $\langle \boldsymbol{\alpha} \rangle_{m,j}$  with Eqs.(57) and (71);
- 16     Calculate second moment of strain field  $\mathbb{K} :: \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{m,j}$  and  $\langle \boldsymbol{\alpha} : \boldsymbol{\alpha} \rangle_{m,j}$  with  
      Eqs.(C.6) and (72);
- 17     Calculate  $\bar{\boldsymbol{\alpha}}_j$  and  $\langle \boldsymbol{\beta} \rangle_j$  with Eqs.(74) and (A.1)
- 18     Calculate  $\theta_j$  and  $\eta_j$  with Eqs.(56) and (59);
- 19     **if**  $\frac{|\delta\theta_j|}{\theta_j} < \epsilon$  **and**  $\frac{|\delta\eta_j|}{\eta_j} < \epsilon,$  **then**
- 20         Return;
- 21     **else**
- 22          $j = j + 1$
- 23      $\bar{\boldsymbol{\sigma}}_{n+1} = \langle \boldsymbol{\sigma}_{n+1} \rangle = f^m \langle \boldsymbol{\sigma}_{n+1} \rangle_m + \sum_{r=1}^N f^{i,r} \langle \boldsymbol{\sigma}_{n+1} \rangle_{i,r};$

348

349 **6.2. Comparisons with direct FEM simulations**

350 The purpose of this section is to verify the accuracy of the BIV model by comparing its pre-  
351 diction with the reference solutions obtained by direct finite element method (FEM) simulations on  
352 the unit cell for two kinds of materials. The first one is a composite material with a non-associated  
353 Drucker-Prager plastic matrix and elastic inclusions (Figure 3(b)), while the second one is a porous  
354 material with non-associated Drucker-Prager plastic matrix and pores. In this section and section 7,  
355 the effective properties of the LCC as well as the field fluctuations are evaluated by using the Hashin-  
356 Shtrikman bounds, i.e., the HS lower bound for the inclusion-reinforced material and the upper bound

357 for the porous material, more details are given in [Appendix C](#). The microstructure of studied mate-  
 358 rials is represented by a periodic assembly of 3D unit cells with spherical inclusion or pore. Taking  
 359 advantage of axial symmetry, the actual hexagonal unit cell is simplified in to a cylinder one and  
 360 only half an axial symmetry plain is considered in the finite element calculations, as illustrated in  
 361 [Figure 3](#). FEM computations are performed using ABAQUS 6.14 using quadratic CAX6 elements  
 362 for inclusion phase and CAX8 elements for matrix phase. Since the focus here is on the modelling of  
 363 non-associated plastic matrix, we assume the interfaces between the inclusions and matrix are perfect  
 364 for the inclusion-reinforced material, implying the interface effects are not taken into account here.  
 365 Note that FEM predictions are labeled “FEM” in the figures. The first- and second-order moments  
 366 of the local fields are computed from direct volume averaging of the local fields in the unit cell ([Yan  
 367 et al., 2007](#)).

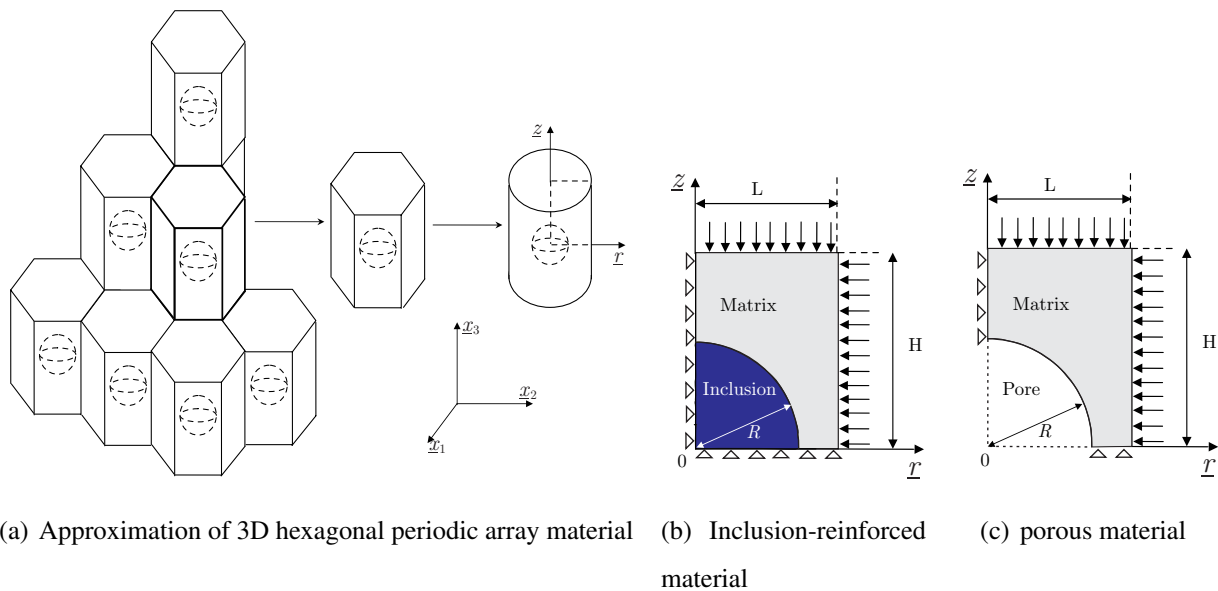


Figure 3: Approximation of 3D hexagonal periodic array with spherical inclusion/pore by axi-symmetric cylinder unit cell

368 For the inclusion-reinforced material, the input parameters for each constituent phase are listed  
 369 in [Tables 1](#) and [2](#). Uniaxial and triaxial compression tests are investigated. The unit cell is first  
 370 subjected to a confining stress (or hydrostatic stress) and then to a differential stress by increasing  
 371 the axial strain in the  $z$  direction. During the differential stress stage, the lateral displacement  $\bar{U}_2$   
 372 is kept uniform along the boundary to satisfy the uniform strain boundary condition. The boundary

373 conditions are illustrated in Figure 3(b) and summarized as follows

$$\left\{ \begin{array}{l} U_3(r, H) = \bar{U}_3, \quad 0 < r < L \\ U_2(L, z) = \bar{U}_2, \quad 0 < z < H \\ U_3(r, 0) = 0, \quad 0 < r < L \\ U_2(0, z) = 0, \quad 0 < z < H \end{array} \right. \quad (75)$$

Table 1: Parameters of solid matrix for composite

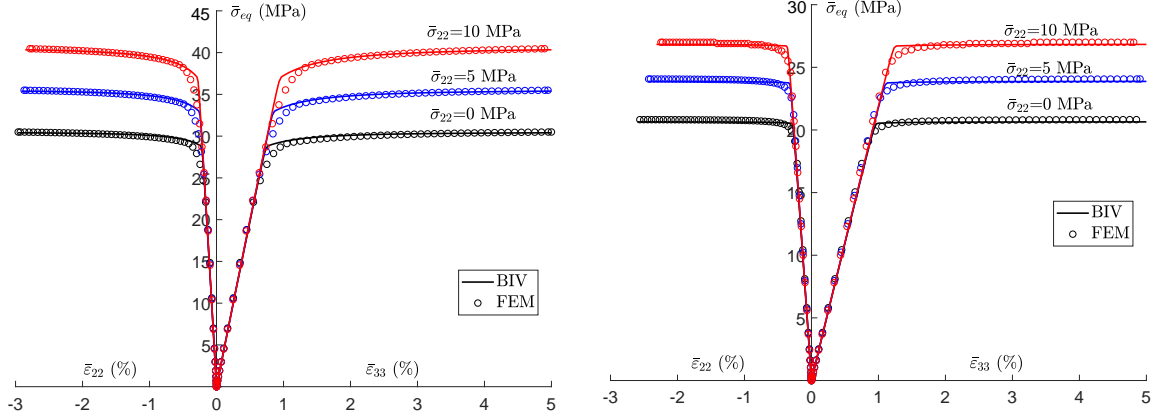
$E^m$ (MPa)	$\nu^m$	$\kappa$	$c$ (MPa)	$\chi_m$
3000	0.3	0.227	30	0.083

Table 2: Parameters of elastic inclusion

$E^i$ (MPa)	$\nu^i$
98000	0.15

374 The parameters for the matrix phase in the porous material are the same as those for the inclusion-  
 375 reinforce composite and listed in Table 1. The boundary conditions on the unit cell are given below  
 376 and illustrated in Figure 3(c).

$$\left\{ \begin{array}{l} U_3(r, H) = \bar{U}_3, \quad 0 < r < L \\ U_2(L, z) = \bar{U}_2, \quad 0 < z < H \\ U_3(r, 0) = 0, \quad R < r < L \\ U_2(0, z) = 0, \quad R < z < H \end{array} \right. \quad (76)$$



(a) Inclusion-reinforced material

(b) Porous material

Figure 4: Macroscopic stress-strain curves for two kinds of heterogeneous materials with non-associated Drucker-Prager perfectly plastic matrix and inclusions/pores ( $f^i = 15\%$ ) in triaxial compression tests with different confining stresses

377 In Figure 4, one shows the macroscopic stress-strain curves for both the inclusion-reinforced  
 378 composite and porous material under uniaxial and triaxial compression tests with different confining  
 379 stresses, respectively obtained by the proposed BIV model and the direct finite element simulations.  
 380 One can observe that the model's predictions coincide very well with the FEM solutions for the all  
 381 cases considered.

382 An example of uniaxial compression test with an unloading-reloading cycle is also studied for the  
 383 inclusion-reinforced composite with  $f^i = 15\%$ . The obtained results are presented in Figure 5. One  
 384 can see the BIV model well reproduces the results given by the FEM simulations.

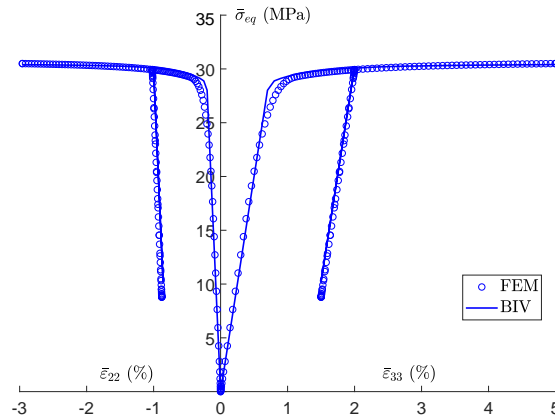


Figure 5: Macroscopic stress-strain curves in uniaxial compression test with an unloading-reloading cycle for the inclusion-reinforced composite with a volume fraction of inclusion of  $f^i = 15\%$

## 385 7. Extension to rocks with isotropic plastic hardening

386 As mentioned that ductile and porous rocks usually exhibit plastic hardening. In the case of  
387 materials considered here, the plastic hardening occurs in the matrix phase. In the context of a  
388 Drucker-Prager plastic criterion, the plastic hardening may leads to an increase of the internal fric-  
389 tion coefficient and hydrostatic tensile strength (related to internal cohesion). However, due to the  
390 strong dissymmetry of strength between compression and tension in most rocks, the tensile strength  
391 is generally small and not affected by the plastic deformation process. The plastic hardening gener-  
392 ally enhances the shear strength through the evolution of the internal frictional coefficient. Therefore,  
393 with the assumption of an isotropic plastic hardening, the internal frictional coefficient of the matrix  
394  $\kappa$  is here assumed to increase during plastic process according to the following law:

$$\kappa(\gamma^p) = \kappa_m - (\kappa_m - \kappa_0) e^{-b_1 \gamma^p} \quad (77)$$

395 where  $\kappa_0$  and  $\kappa_m$  denote the initial threshold and the asymptotic value of the frictional coefficient  
396 respectively, while  $b_1$  is a parameter controlling the plastic hardening rate.

397 On the other hand, the plastic dilatancy coefficient  $\chi$  can also evolve with the plastic deforma-  
398 tion history, translating the transition from plastic compressibility to dilatancy. Therefore, we here  
399 consider that  $\chi$  is also a function of  $\gamma^p$  through the following relation

$$\chi(\gamma^p) = \chi_m (1 - e^{-b_2 \gamma^p}) \quad (78)$$

400 where  $\chi_m$  is the asymptotic value of the plastic dilatancy coefficient, and  $b_2$  is a parameter controlling  
401 its evolution.

402 In order to fully account for this kind of plastic hardening law in the proposed BIV model, the  
403 thermodynamics formulation presented above should be modified by considering the evolution of  
404 elastic domain during plastic deformation process. **However, due to the fact that the plastic hardening  
405 is described by the evolution of the friction coefficient, the evolution measurement of elastic domain  
406 cannot be represented by a constant force variable but by a function of mean stress.** This render the  
407 mathematical treatment of the BIV model very complicated. In order to avoid this complex mathe-  
408 matical difficulty and provide a pragmatcal model being easy to be implemented, we shall propose a  
409 heuristic extension of the BIV model formulated above for materials without plastic hardening. Ac-  
410 cording to the theoretical formulation presented in Sections 3 and 4, when the values  $\kappa$ ,  $c$  and  $\chi$  are  
411 constant, the average secant viscosity function of solid matrix  $\eta$  is given in Eq.(59). We here assume  
412 that this result remains applicable for the solid matrix where the values of  $\kappa$  and  $\chi$  are step by step



413 updated at each loading increment. Therefore, we propose an explicit incremental hardening scheme.  
 414 The average secant viscosity function and the plastic dilatancy coefficient  $\chi$  at the loading increment  
 415  $n + 1$  is approximated as follows (for the sake of simplicity, the increment number  $n + 1$  is omitted in  
 416 the following equations):

$$\eta = -\frac{\kappa(\langle\gamma_n^p\rangle_m)(\langle\sigma_m\rangle_m - c)}{\dot{\bar{\alpha}}} \quad (79)$$

$$\chi(\langle\gamma_n^p\rangle_m) = \chi_m(1 - e^{-b_2\langle\gamma_n^p\rangle_m}) \quad (80)$$

417 In these relations,  $\langle\gamma_n^p\rangle_m$  is the average value of equivalent plastic shear strain in the solid matrix  
 418  $\gamma^p$  calculated by Eq.(A.2) at the end of the loading increment  $n$  and its value if frozen during the  
 419 current increment  $n + 1$ . Accordingly, the values of frictional coefficient  $\kappa$  and plastic dilatancy  
 420 coefficient  $\chi$  are also frozen to those calculated at the end of the previous increment such as  $\kappa(\langle\gamma_n^p\rangle_m)$   
 421 and  $\chi(\langle\gamma_n^p\rangle_m)$ . Therefore, the solid matrix is treated as a perfectly plastic material during the current  
 422 loading increment.

### 423 7.1. Comparisons with direct FEM simulations

424 The accuracy of the heuristically extended BIV model for materials with an isotropic hardening  
 425 is now checked by comparing the model's predictions with direct FEM simulations for both local  
 426 and macroscopic responses. Two kinds of materials are again studied: inclusion-reinforced com-  
 427 posites and porous materials. Conventional triaxial compression tests are considered. The boundary  
 428 conditions for the two materials are the same as those presented in Section 6.2. The following in-  
 429 put parameters are selected for the isotropic hardening law:  $\kappa_0 = 1 \times 10^{-5}$ ,  $\kappa_m = 0.227$ ,  $b_1 = 140$ ,  
 430  $\chi_m = 0.083$  and  $b_2 = 70$ .

#### 431 7.1.1. Inclusion-reinforced composites

432 Two volume fractions of elastic inclusions are considered:  $f^i = 5\%$  and  $f^i = 15\%$ . In Figure 6,  
 433 one shows the macroscopic stress-strain curves in the uniaxial compression test, respectively obtained  
 434 by the BIV model and FEM simulations. It can be seen that there is a good agreement between these  
 435 two results. In Figure 7, we emphasize the volume strain evolution  $\bar{\epsilon}_v$  as a function of axial strain  $\bar{\epsilon}_{33}$   
 436 with different values of the maximum dilatancy coefficient  $\chi_m$  and for  $f^i = 15\%$ . It is noticed that the  
 437 proposed BIV model is able to well reproduce the volume compressibility-dilatancy transition which  
 438 is an important property of rocks. More precisely, the volumetric dilatancy is enhanced when the  
 439 value of  $\chi_m$  increases. The results due to the BIV model well coincident with the FEM simulations.

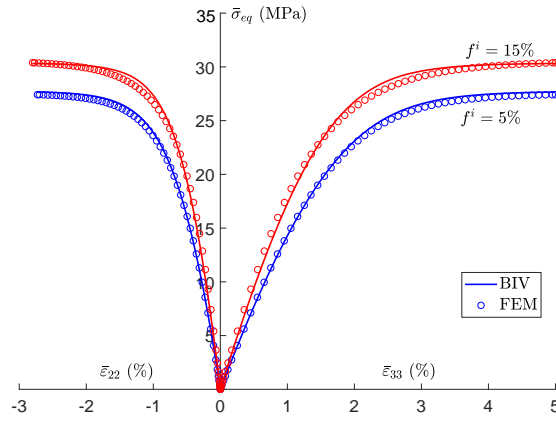


Figure 6: Macroscopic stress-strain curves in uniaxial compression test for an inclusion-reinforced composite with two volume fractions of inclusions ( $f^i = 5\%$  and  $f^i = 15\%$ )

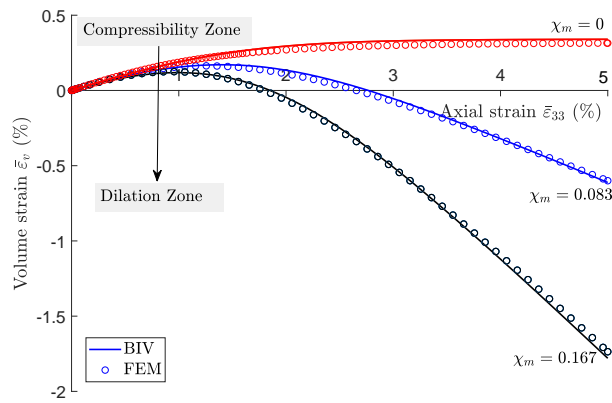


Figure 7: Evolution of macroscopic volumetric strain in uniaxial compression test for different values of plastic dilatancy coefficient  $\chi$  for an inclusion-reinforced composite with a volume fraction of inclusions of  $f^i = 15\%$

440 Moreover, the proposed BIV model is also able to capture another important property of geolog-  
 441 ical materials, which is the influence of confining stress on the macroscopic behavior. This is clearly  
 442 illustrated in Figure 8. The stress-strain curves are presented for the uniaxial compression test and  
 443 two triaxial compression tests respectively with a different confining stress of 10MPa and 20MPa.  
 444 Again, the BIV predictions are in good agreement with the FEM solutions.

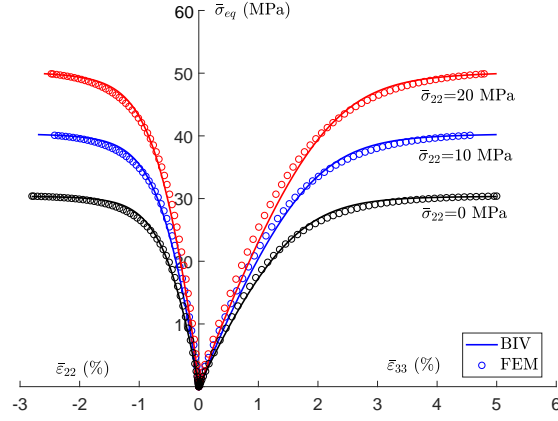
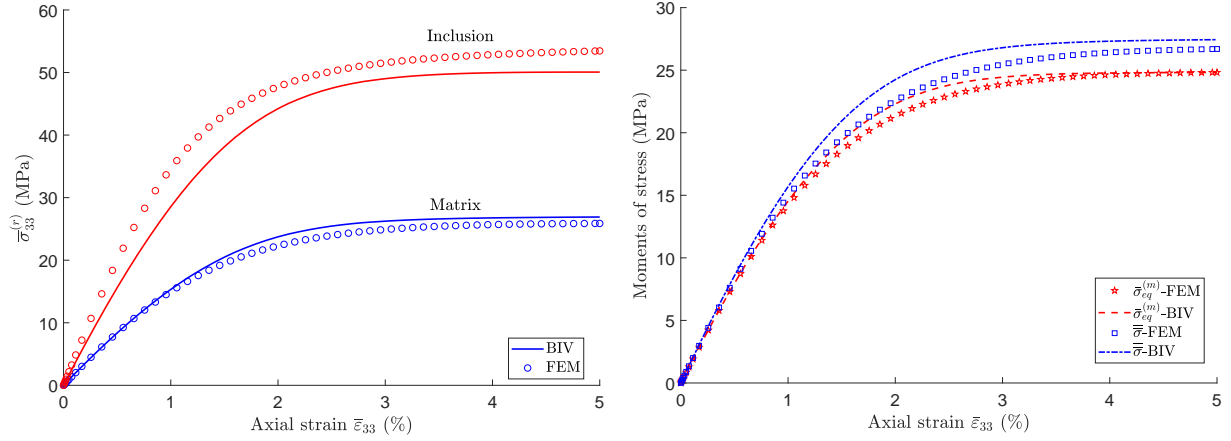
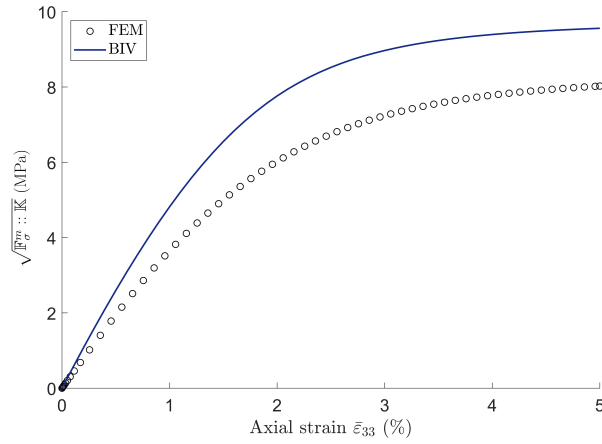


Figure 8: Macroscopic stress-strain curves in uniaxial and triaxial compression tests with two different confining stresses two for an inclusion-reinforced composite with  $c^{(2)} = 15\%$

445 In order to further assess the accuracy of the BIV model, the evolution of local stresses during the  
446 loading history is also investigated for the case of uniaxial compression test and of an inclusion vol-  
447 ume fraction of  $f^i = 15\%$ . For instance, the evolutions of average stress respectively in the inclusion  
448 and matrix phases are presented in Figure 9(a). In Figure 9(b), one presents the evolutions of the dif-  
449 ferent denominators  $\bar{\sigma}_{eq}^m$  and  $\bar{\bar{\sigma}}$ , respectively related to the first-order and second-order moments of the  
450 local stress field over the plastic matrix. Lastly, in Figure 9(c), the evolution of the stress fluctuation  
451  $\sqrt{\mathbb{F}_{\sigma}^m :: \mathbb{K}}$  in the matrix is presented. It is observed that the BIV model provides an accurate prediction  
452 for the evolution of average stress within the matrix, while a less accurate prediction regarding the  
453 average stress in the inclusion phase (Figure 9(a)). The BIV results are also in good agreement with  
454 the FEM solutions for the stress moments  $\bar{\sigma}_{eq}^m$  and  $\bar{\bar{\sigma}}$  (Figure 9(b)). Lastly, although the BIV model  
455 overestimates the stress fluctuation within the matrix, it is still able to reproduce the good evolution  
456 trend of FEM solutions (Figure 9(c)).



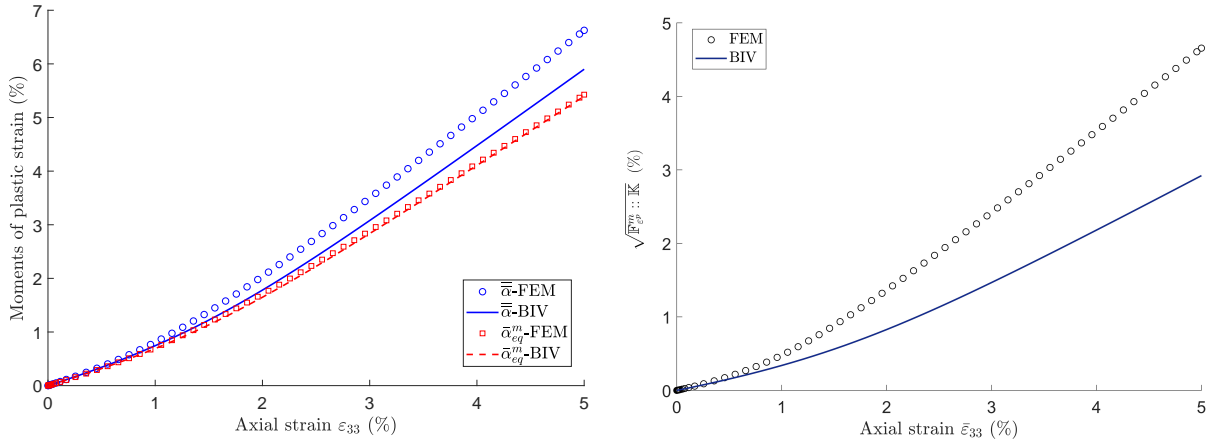
(a) Evolution of average stress in constituent phases versus macroscopic axial strain (b) First and second moments of stress over matrix



(c) Fluctuations of stress over matrix

Figure 9: Local stress responses in uniaxial compression test for an inclusion-reinforced composite with  $f^i = 15\%$

457 On the other hand, the evolution of the local plastic strain is also studied. In Figure 10(a), one can  
 458 find a quite good agreement between the BIV result and FEM solution for the first-order moment of  
 459 local plastic strain field over the matrix  $\bar{\alpha}_{eq}^m$ . However, it seems that the BIV model underestimates the  
 460 second-order moment of plastic strain in the matrix  $\bar{\bar{\alpha}}$ . The fluctuation of plastic strain field is shown  
 461 in Figure 10(b). The BIV model is able to capture the trend of the FEM solution although there exist  
 462 some scatters between them.



(a) First and second moments of plastic strain over matrix

(b) Fluctuation of plastic strain over matrix

Figure 10: Local plastic strain responses in uniaxial compression test of an inclusion-reinforced composite with  $f^i = 15\%$

### 463 7.1.2. Porous material

464 The macroscopic stress-strain curves in uniaxial compression test with two values of porosity  $f^i =$   
 465 15% and 5% are presented in Figure 11. There is a good agreement between the BIV predictions and  
 466 FEM results. Furthermore, the stress-strain curves in triaxial compression tests with three different  
 467 confining stresses are presented in Figure 12 for a porosity of  $f^i = 15\%$ . Once more, the BIV model  
 468 correctly captures the effect of confining stress and well reproduces the FEM solutions.

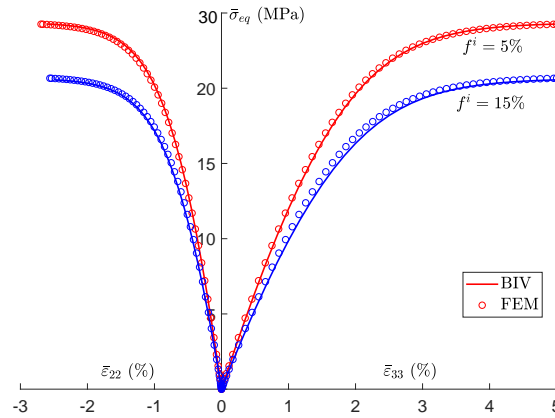


Figure 11: Macroscopic stress-strain curves in uniaxial compression test for a porous material with two different values of porosity ( $f^i = 5\%$  and  $f^i = 15\%$ )

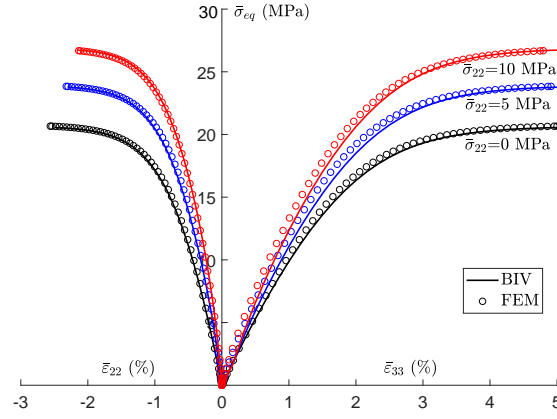
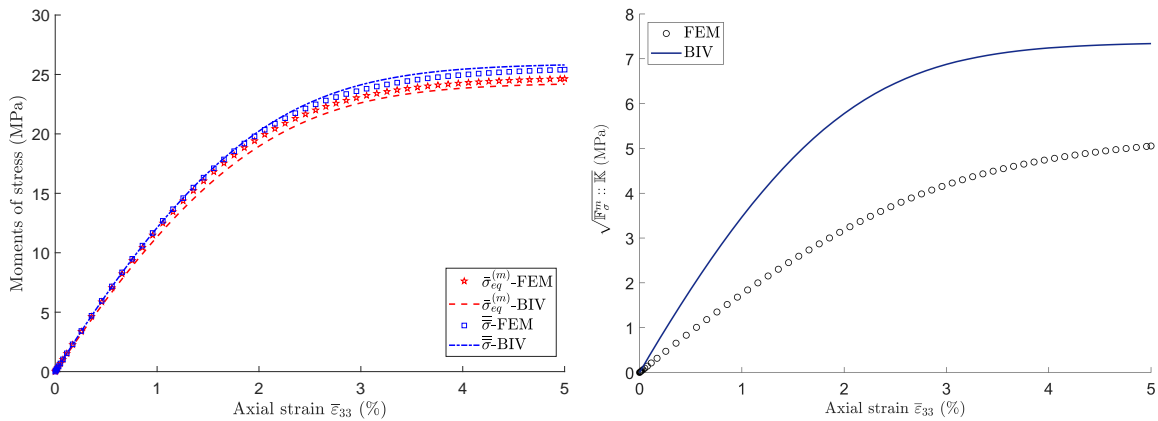


Figure 12: Macroscopic stress-strain curves in triaxial compression tests with three different confining stresses for a porous material with a porosity of  $f^i = 15\%$

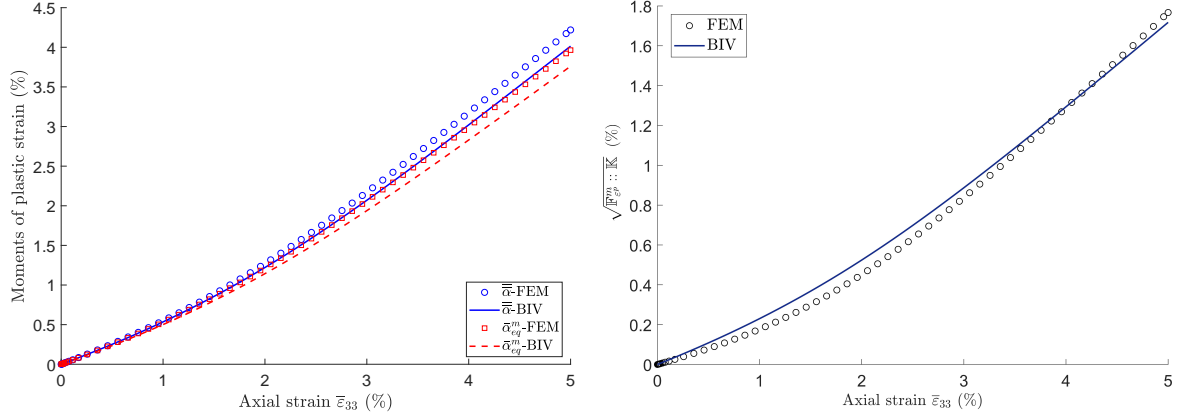
469 As for the inclusion-reinforced composite, the local stress and strain responses of porous material  
 470 are also investigated for the case of uniaxial compression test and with a porosity of  $f^i = 15\%$ . In  
 471 Figure 13(a), the evolutions of the first and second-order moments of local stress field over the matrix,  
 472  $\bar{\sigma}_{eq}^m$  and  $\bar{\bar{\sigma}}$ , are depicted. The evolution of the stress fluctuations is given in Figure 13(b). One can  
 473 find a similar trend as that already obtained in Figure 9 for the inclusion-reinforced composite. The  
 474 evolutions of the moments and fluctuations of local plastic strain field over the matrix are shown in  
 475 Figure 14. As shown in Figure 14(a), although the BIV model qualitatively reproduces the trend of  
 476 the FEM solutions, it slightly underestimates the denominators  $\bar{\alpha}_{eq}^m$  and  $\bar{\bar{\alpha}}$ . Compared with Figures  
 477 14(b) and 10(b), the fluctuations of the plastic strain field are now better captured by the BIV model  
 478 for the porous material than for the inclusion-reinforced composite.



(a) First- and second-order moments of stress over matrix

(b) Fluctuations of stress over matrix

Figure 13: Local stress responses in uniaxial compression test for a porous material with a porosity  $f^i = 15\%$



(a) First and second-order moments of plastic strain over matrix (b) Fluctuations of plastic strain over matrix

Figure 14: Local plastic strain responses in uniaxial compression test for a porous material with a porosity of  $f^i = 15\%$

## 479 7.2. Application examples

480 In this section, two application examples are presented to show the ability of the extended bi-  
 481 potential based incremental variational model to reproduce experimental responses of two typical  
 482 rocks: the Callovo-Oxfordian claystone and Vosges sandstone.

### 483 7.2.1. Application to Callovo-Oxfordian claystone

484 The Callovo-Oxfordian claystone has been extensively investigated in France as a potential geo-  
 485 logical barrier for the underground disposal of nuclear waste (Armand et al., 2016). It is a sedimentary  
 486 rock with complex multi-scale structures (Robinet, 2008). At the micrometer scale, this clayey rock  
 487 is composed of a quasi-continuous clay matrix in which mineral grains, mainly quartz and calcite  
 488 grains, are embedded. The clay matrix can exhibit important plastic deformation (Guéry et al., 2008,  
 489 2010). For the sake of simplicity, the behavior of clay matrix is here described by an isotropic elastic-  
 490 plastic model. The linear Drucker-Prager criterion is adopted together with an isotropic hardening  
 491 law and a non-associated plastic flow rule. On the other hand, for the range of stresses considered in  
 492 the application, the mechanical behavior of the quartz and calcite grains can be reasonably described  
 493 by a linear elastic model. Furthermore, as the elastic properties of calcite and quartz are quite similar,  
 494 for the sake of simplicity, they are seen a single phase of elastic inclusions.

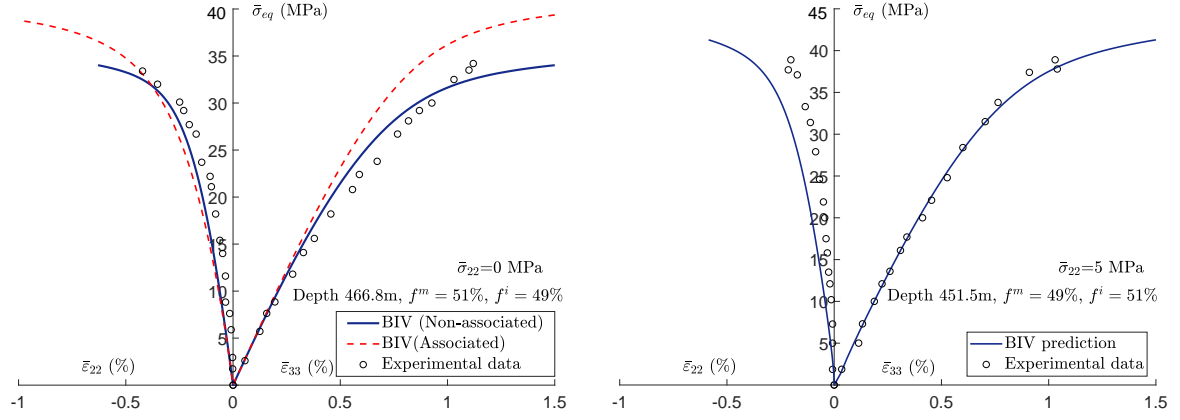
495 The preliminary challenge of the application of the micro-mechanical model is the identification  
 496 of local parameters for each constituent phase. To this end, the local mechanical behavior should  
 497 be determined. This direct identification method is so far not possible because relevant data on me-  
 498 chanical responses at the microscopic scale are not fully available. Here an indirect identification

499 procedure is employed here. The elastic coefficients of the effective elastic inclusion phase are taken  
500 as the volumetric average values of the quartz and calcite grains (Jiang et al., 2009). Note that the  
501 elastic coefficients of quartz and calcite grains elastic properties of calcite and quartz grains are well  
502 known and can be obtained from existing data(Lide, 2004). It is easily to obtain the Young's mod-  
503 ulus and Poisson's ratio of the effective elastic inclusion are equal to  $E^i = 98\text{GPa}$  and  $\nu^i = 0.15$ .  
504 However, the elastic coefficients of the clay matrix are not available from direct experimental mea-  
505 surement. They are calibrated here by an inverse homogenization procedure (Guéry et al., 2008), from  
506 the macroscopic elastic coefficients obtained in triaxial compression tests on the samples with known  
507 mineralogical compositions (Chiarelli, 2000). We calculate the typical values of Young's modulus  
508  $E^m = 3\text{GPa}$  and Poisson's ratio  $\nu^m = 0.3$ . On the other hand, the values of plastic parameters of  
509 clay matrix are fitted by a numerical optimization of macroscopic stress-strain curves obtained by  
510 convention laboratory tests (conventional triaxial compression tests, proportional compression tests,  
511 lateral extension test, etc.) for a chosen mineralogical composition similar to that proposed in (Guéry  
512 et al., 2008, Shen et al., 2012). The obtained values are then fixed and applied to samples with dif-  
513 ferent mineralogical compositions. The obtained plastic parameters values are given as:  $\kappa_0 = 10^{-5}$ ,  
514  $\kappa_m = 0.283$ ,  $b_1 = 250$ ,  $\chi_m = 0.05$ ,  $b_2 = 50$ ,  $c = 20\text{MPa}$ .

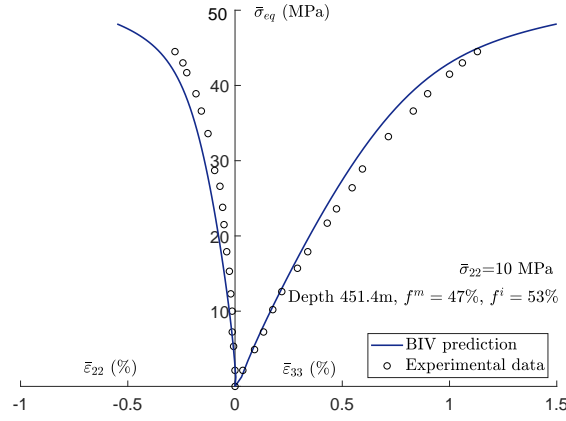
515 The mechanical responses of the claystone are now studied using the proposed BIV model in  
516 triaxial compression tests, proportional compression tests and lateral extension tests. It is noteworthy  
517 that these tests were performed on samples coming from different geological depths ranging from  
518 415.4m to 482.4m, with different mineral compositions. However, a sole set of parameters is used for  
519 the modeling of different tests on different samples.

520 In Figure 15, the stress-strain curves of claystone in triaxial compression tests are presented. One  
521 observes a good agreement between model's predictions and experimental data. The BIV model is  
522 able to well reproduce the main features of the claystone mechanical behavior in this loading path,  
523 such as the volume compressibility-dilatancy and confining stress sensitivity. The impact of miner-  
524 alogical compositions is also correctly taken into account. Further, in Figure 15(a), the numerical  
525 results respectively provided by the associated and non-associated plastic model are compared. It is  
526 clear that the non-associated model gives a better prediction than the associated one.





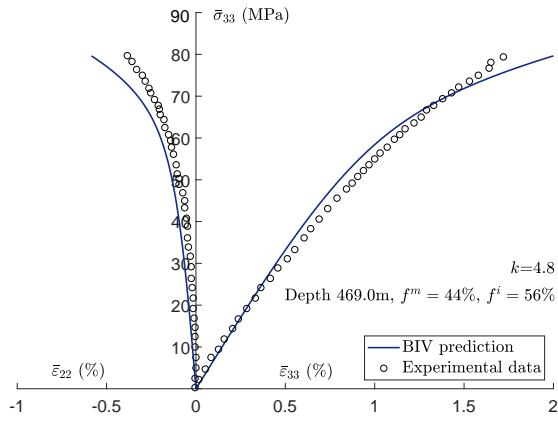
(a) Depth 466.8m,  $f^m = 51\%$ ,  $f^i = 49\%$ ,  $\bar{\sigma}_{22} = 0$  MPa (b) Depth 451.5m,  $f^m = 49\%$ ,  $f^i = 51\%$ ,  $\bar{\sigma}_{22} = 5$  MPa



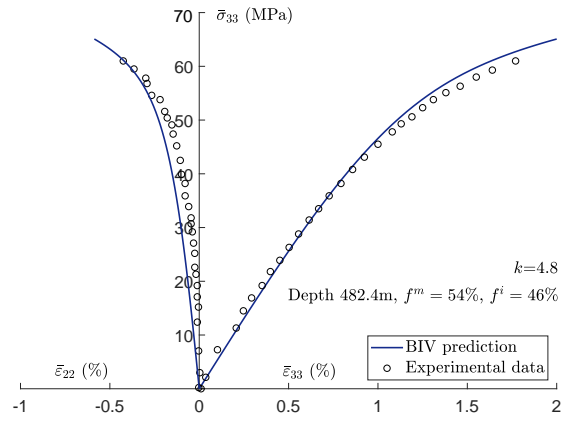
(c) Depth 451.4m,  $f^m = 47\%$ ,  $f^i = 53\%$ ,  $\bar{\sigma}_{22} = 10$  MPa

Figure 15: Comparison of stress-strain curves between experimental data and numerical results in triaxial compression tests on Callovo-Oxfordian claystone samples with different mineralogical compositions

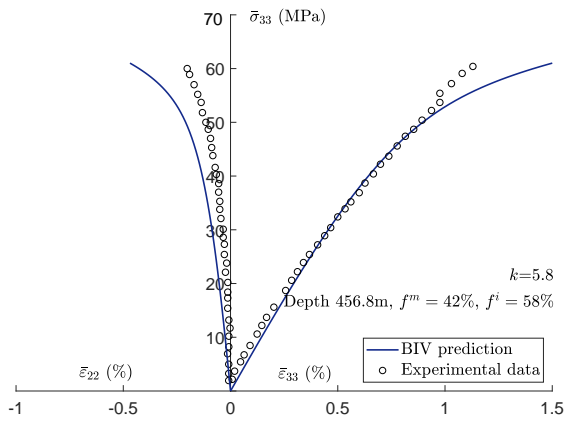
527 For providing a complementary validation of the BIV model, proportional compression and lateral  
 528 extension tests are also studied. In a proportional compression test, the axial stress  $\bar{\sigma}_{33}$  and confining  
 529 stress  $\bar{\sigma}_{11}$  are simultaneously increased with a constant ratio  $k = \frac{\bar{\sigma}_{33}}{\bar{\sigma}_{11}}$ . In a lateral extension test, the  
 530 sample is first subjected to a hydrostatic stress state to a desired value, and then the lateral stress  
 531  $\bar{\sigma}_{11}$  is progressively decreased while the axial stress  $\bar{\sigma}_{33}$  is kept constant. The comparisons between  
 532 numerical predictions and experimental data for these two kinds of tests are shown in Figure 16 and  
 533 17, respectively. Again, one gets a good general agreement and the BIV model correctly reproduces  
 534 the main characteristics of mechanical responses of the claystone in these two loading paths.



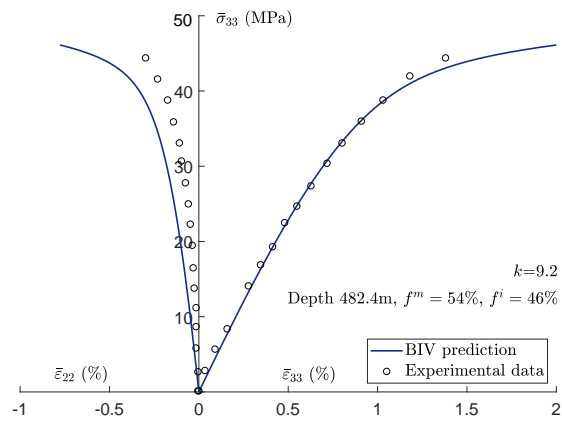
(a) Depth 469.0m,  $f^m = 44\%$ ,  $f^i = 56\%$ ,  $k = 4.8$



(b) Depth 482.4m,  $f^m = 54\%$ ,  $f^i = 46\%$ ,  $k = 4.8$



(c) Depth 456.8m,  $f^m = 42\%$ ,  $f^i = 58\%$ ,  $k = 5.8$



(d) Depth 482.4m,  $f^m = 54\%$ ,  $f^i = 46\%$ ,  $k = 9.2$

Figure 16: Comparisons of mechanical responses between experimental data and numerical results in proportional compression tests on Callovo-Oxfordian claystone with different mineralogical compositions

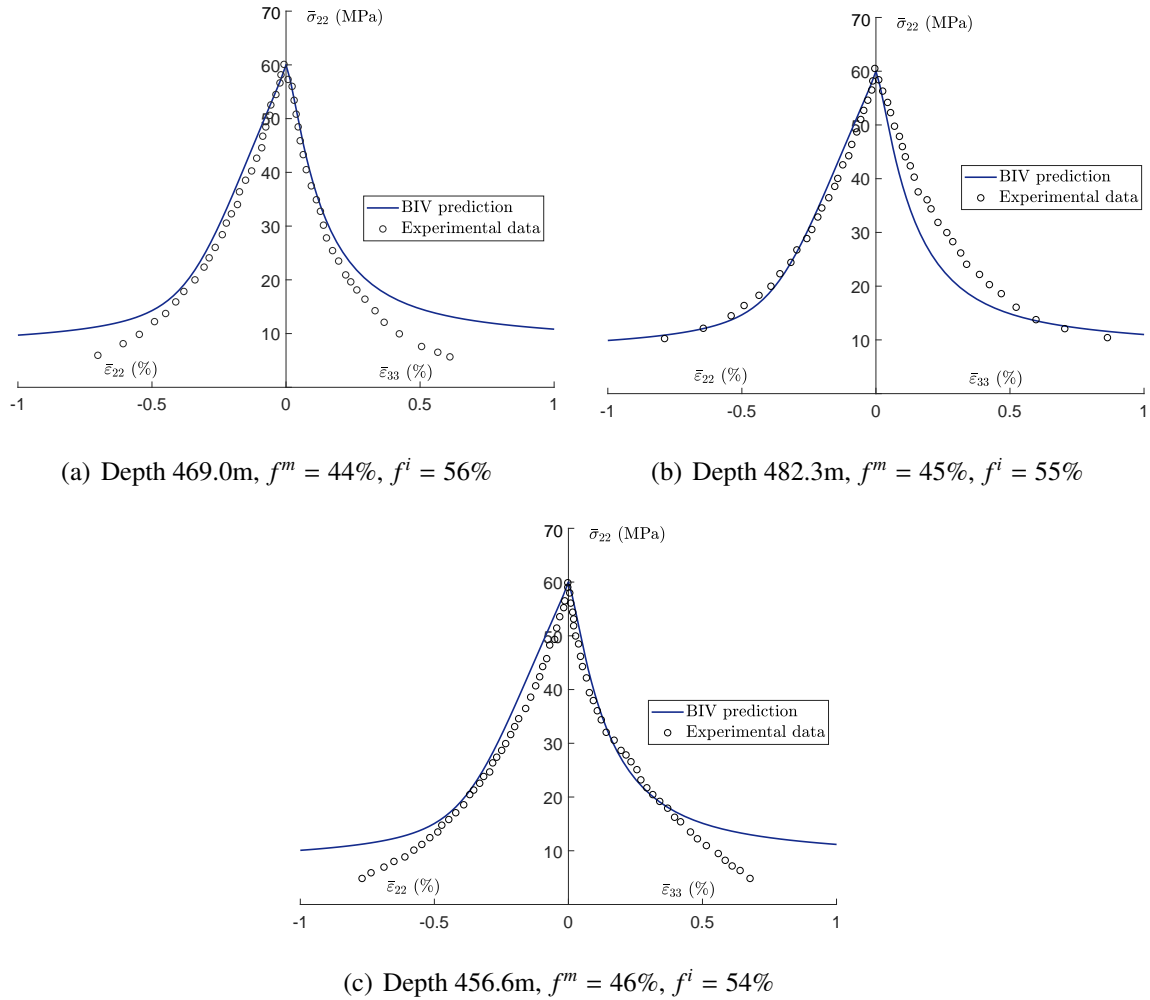


Figure 17: Comparisons of mechanical responses between experimental data and numerical results in lateral extension tests with an initial confining stress of 60MPa on Callovo-Oxfordian claystone with different mineralogical compositions

### 535 7.2.2. Application to Vosges sandstone

536 The Vosges sandstone is here studied as a typical porous rock. Its microstructure and macro-  
 537 scopic behaviors have been investigated in a number of previous studies, for instance (Khazraei, 1996,  
 538 Bésuelle et al., 2000). The average porosity is about 20% and the solid matrix is composed of nearly  
 539 93% quartz grains with a few percent of feldspar and white mica. As a first approximation, the sand-  
 540 stone can be considered as an isotropic material. The mechanical strength of the sandstone strongly  
 541 depends on confining pressure. In this study, the solid matrix is described by a non-associated plastic  
 542 model based on the Drucker-Prager criterion. The elastic and plastic parameters of solid matrix are  
 543 not directly measured but also indirectly estimated. The elastic coefficients can be easily identified by  
 544 an inverse homogenization procedure from measured macroscopic values and the known porosity of  
 545 sample. The plastic parameters are again fitted from a numerical optimization procedure of macro-  
 546 scopic stress-strain curves for a given porosity. The obtained values of parameters are given in Table

Table 3: Parameters of solid matrix for porous Vosges sandstone

$E^m$ (GPa)	$\nu^m$	$\kappa_0$	$\kappa_m$	$c$ (MPa)	$b_1$	$\chi_m$	$b_2$
40	0.25	$10^{-5}$	0.433	40	900	0.333	500

548 In Figure 18, we first present the stress-strain curves in conventional triaxial compression tests  
549 with four different confining stresses from 5MPa to 40MPa. Like the claystone, there is a good  
550 agreement between model's predictions and experimental data. The effect of confining stress on  
551 macroscopic response is well captured. However, the mechanical strength of sandstone is slightly  
552 overestimated by the model for the test with a low confining stress of 5MPa. This is due to the fact  
553 that the linear Drucker-Prager criterion used for the solid matrix is not well adopted in the zone of  
554 low mean stress and tensile stress. The use of a curved yield surface for the solid matrix, for example  
555 the Mises-Schleicher criterion, would improve numerical results. In Figure 18(b), one can see that the  
556 non-associated model provides a better prediction of lateral strain than the associated model. However,  
557 unlike the result of claystone shown in Figure 15(a), the non-associated flow rule coefficient has no  
558 influence on the peak strength of porous sandstone.

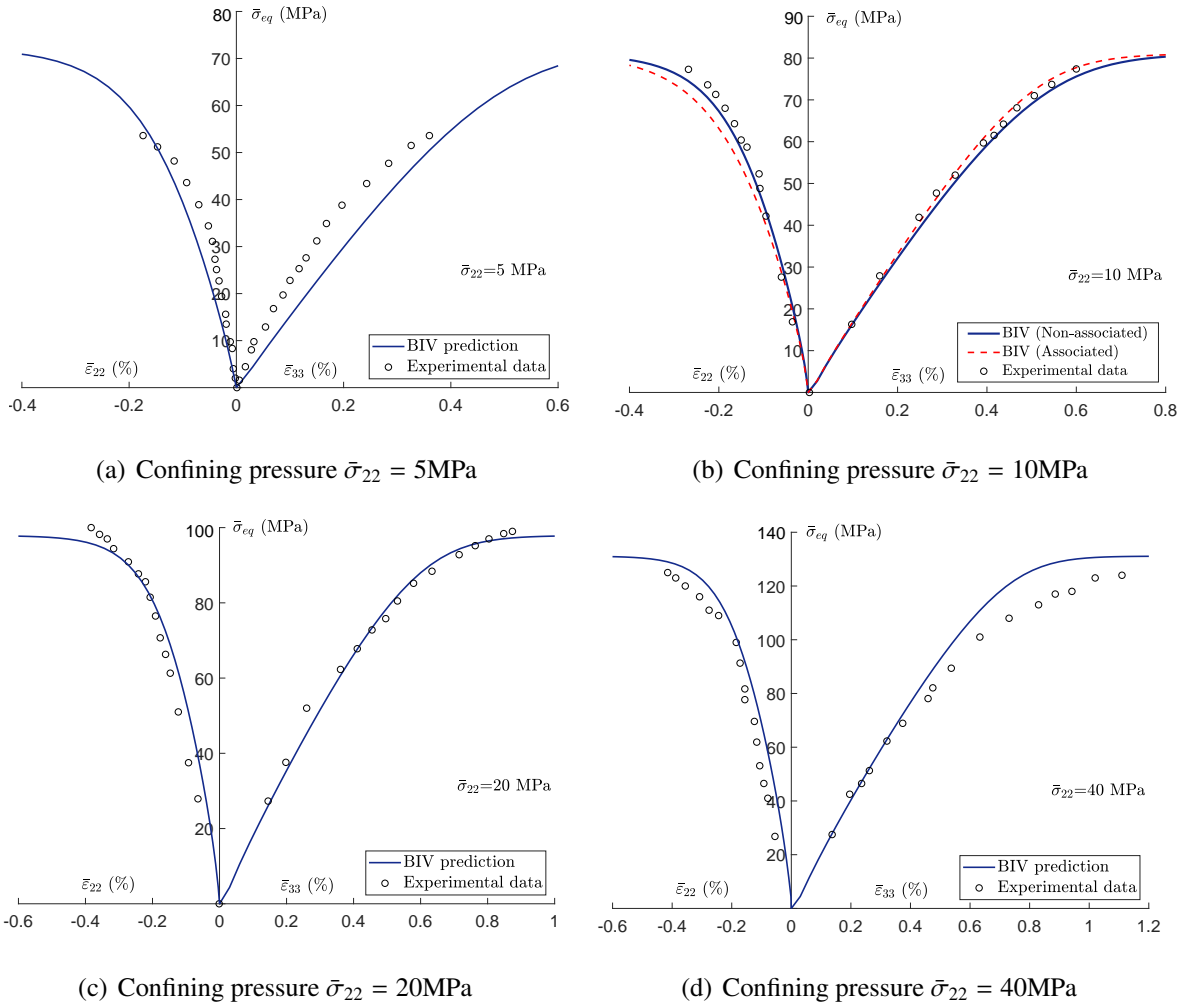


Figure 18: Comparisons of mechanical responses between experimental data and numerical results in triaxial compression tests on Vosges sandstone

559 The mechanical responses of Vosges sandstone in proportional compression and lateral extension  
 560 tests are presented in Figures 19 and 20 respectively. Once more, it is found that the proposed BIV  
 561 model well reproduce experimental data for these loading paths. In particular, as shown in Figure 19,  
 562 the transition from volumetric compressibility to dilatancy is well reproduced by the BIV model due  
 563 to the non-associated plastic flow rule used for the solid matrix.

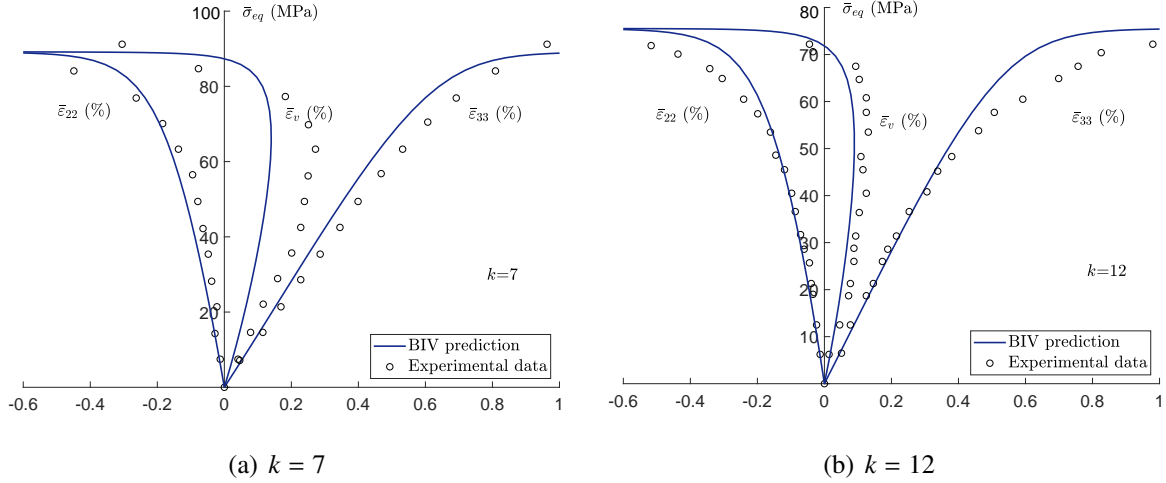


Figure 19: Comparison of stress-strain curves between experimental data and numerical results for proportional compression tests on Vosges sandstone

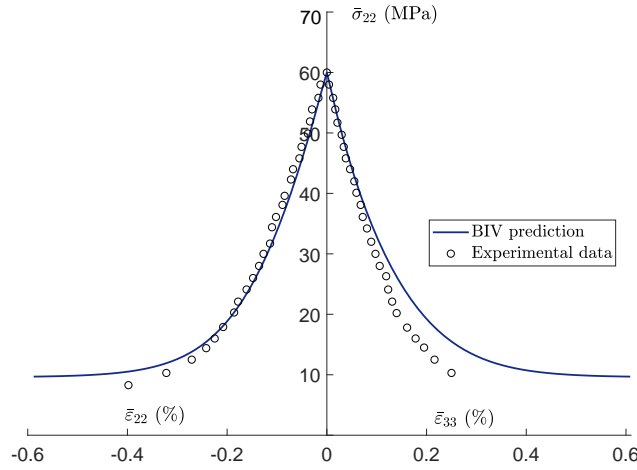


Figure 20: Comparison of mechanical response between experimental data and numerical results for lateral extension test on Vosges sandstone with an initial confining pressure of 60MPa and axial stress of 90MPa

## 564 8. Concluding remarks

565 In this paper, we have developed a new incremental variational framework for the estimation of  
 566 effective elastic-plastic properties of a class of heterogeneous rocks by using the bi-potential theory.  
 567 These materials are considered as implicit standard materials (ISMs). In particular, a bi-potential  
 568 based incremental variational model (BIV) has been formulated for those rocks with a non-associated  
 569 plastic matrix described by a Drucker-Prager type yield function and an isotropic hardening law.

570 The BIV model has first been formulated by considering an elastic perfectly plastic matrix phase.  
 571 With the help of the bi-potential theory, we have determined the local incremental elastic and plastic  
 572 bi-potentials of the matrix. We have also introduced an appropriate optimization method for the

573 estimation of the effective incremental bi-potential and macroscopic stress. The accuracy of BIV  
574 model has been demonstrated through the comparisons with direct finite element simulations for both  
575 inclusion-reinforced composites and porous materials.

576 A heuristic extension of the BIV model has then been proposed in view of estimating effective  
577 behaviors of heterogeneous rocks exhibiting an isotropic plastic hardening. This has been done by  
578 assuming that the general incremental variational formulation obtained the perfectly plastic matrix re-  
579 mains applicable at each loading increment if the plastic hardening variables and functions are frozen.  
580 The plastic hardening has been taken into account by updating the values of the frozen hardening func-  
581 tions at each loading increment. The efficiency of the heuristically extended BIV model has also been  
582 confirmed by the comparisons with direct finite element simulations for both inclusion-reinforced  
583 composites and porous materials. It has been found that the BIV model was able to provide a good  
584 estimation of the fluctuations of local stress and plastic strain fields. However, the average stress  
585 in the inclusion phase was underestimated for the inclusion-reinforced composites while the stress  
586 fluctuation in the matrix phase is overestimated for both materials. Therefore, some improvement  
587 remains needed, for example, by using a second-order comparison composite for the estimation of  
588 incremental bi-potential of the plastic matrix.

589 Finally, the BIV model has been applied to studying the mechanical behavior of two typical ge-  
590 ological materials, the Callovo-Oxfordian claystone and Vosges sandstone, under different loading  
591 paths. In a general way, the numerical results are in good agreement with experimental data. The  
592 main features of mechanical behaviors of two materials are correctly reproduced by the BIV model,  
593 such as influence of confining stress and volume compressibility-dilatancy transition.

594 In this work, we have focused on the short-term mechanical behavior of dry materials. In future,  
595 the BIV model is expected to be extended to the time-dependent behavior and to saturated and un-  
596 saturated materials. **Moreover, it is acknowledged that the interfaces between the inclusions and the  
597 matrix play a non-negligible role in rocks plastic deformation and damage. The effects of interface  
598 will be also taken into account in our future work.**

## 599 **Acknowledgment**

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603 Science Foundation funded project(Grant Nos. 2020M682638, 2020M682707).

604 **Appendix A. Approximation of the local elastic bi-potential (24)**

605 Inspired by Boudet et al. (2016), we assume that the volumetric plastic strain field  $\boldsymbol{\beta}$  and the inter-  
 606 nal variable field  $\gamma^p$  are constant values in the solid matrix, denoted by  $\langle \boldsymbol{\beta} \rangle_m$  and  $\langle \gamma^p \rangle_m$ , respectively.  
 607 For the local stress state situated on the regular part of Drucker-Prager yield surface, the evolution of  
 608  $\langle \boldsymbol{\beta} \rangle_m$  and  $\langle \gamma^p \rangle_m$  can be expressed as follows by taking into account Eq. (31):

$$\langle \boldsymbol{\beta} \rangle_m = \langle \boldsymbol{\beta}_n \rangle_m + \overline{\dot{\boldsymbol{\alpha}}} \Delta t \chi \boldsymbol{\delta} \quad (\text{A.1})$$

$$\langle \gamma^p \rangle_m = \langle \gamma_n^p \rangle_m + \overline{\dot{\boldsymbol{\alpha}}} \Delta t \quad (\text{A.2})$$

609 where  $\langle \boldsymbol{\beta}_n \rangle_m$  and  $\langle \gamma_n^p \rangle_m$  are the volume average values of fields  $\boldsymbol{\beta}$  and  $\gamma$  over the matrix phase at the  
 610 step  $n$ , and

$$\overline{\dot{\boldsymbol{\alpha}}} = \frac{1}{\Delta t} \sqrt{\frac{2}{3} \langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) : (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) \rangle_m} = \frac{1}{\Delta t} \overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n} \quad (\text{A.3})$$

611 Accordingly, one gets:

$$b_e^m(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}) \simeq b_e^{app}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{\sigma} : \mathbb{S}^m : \boldsymbol{\sigma} + \frac{1}{2} \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n} \chi \boldsymbol{\delta} \right) : \mathbb{C}^m : \left( \boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta}_n \rangle_m - \overline{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n} \chi \boldsymbol{\delta} \right) \quad (\text{A.4})$$

612 **Appendix B. Minimization of  $J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$**

613 By making use of the minimization of  $J_0^m(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$  w.r.t.  $\boldsymbol{\alpha}$ , and after taking into account the relation  
 614 (44) of  $J_0^m$ , one gets,

$$\frac{\partial J_0^m}{\partial \boldsymbol{\alpha}} = -\mathbb{K} : \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) - \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) \frac{\partial \langle \boldsymbol{\beta} \rangle_m}{\partial \boldsymbol{\alpha}} + 2 \frac{\eta_p \theta}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) = 0 \quad (\text{B.1})$$

615 It is noticed that Eq. (53) in its field form can be rewritten as:

$$\theta (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) = (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) \quad \forall \underline{x} \in \Omega_m \quad (\text{B.2})$$

616 Considering the expression (A.1) and (B.2), one obtains

$$\frac{\partial \langle \boldsymbol{\beta} \rangle_m}{\partial \boldsymbol{\alpha}} = \frac{2\chi\theta}{3\Delta t \overline{\dot{\boldsymbol{\alpha}}}} \boldsymbol{\delta} \otimes (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \quad (\text{B.3})$$

617 then

$$-\mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) : \frac{\partial \langle \boldsymbol{\beta} \rangle_m}{\partial \boldsymbol{\alpha}} = 2 \frac{\eta_{cp} \theta}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \quad (\text{B.4})$$

618 with

$$\eta_{cp} = \frac{-3\chi\sigma_m}{3\overline{\dot{\boldsymbol{\alpha}}}}, \quad \sigma_m = \frac{1}{3} \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) : \boldsymbol{\delta} \quad (\text{B.5})$$



619 For ease of calculation, we assume that  $\eta_{cp}$  takes its average value in the matrix phase, i.e.:

$$\eta_{cp} = \frac{-3\chi \langle \sigma_m \rangle_m}{3\bar{\dot{\alpha}}} \quad (\text{B.6})$$

620 Substituting Eqs. (B.2) and (B.4) into (B.1), ont gets:

$$\frac{\partial J_0^m}{\partial \alpha} = -\mathbb{K} : \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) + 2 \frac{\eta \theta}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) = 0 \quad (\text{B.7})$$

621 with

$$\eta = \eta_p + \eta_{ih} + \eta_{cp} = \frac{\langle \sigma_y \rangle_m - 3\chi \langle \sigma_m \rangle_m}{3\bar{\dot{\alpha}}} = -\frac{\kappa (\langle \sigma_m \rangle_m - c)}{\bar{\dot{\alpha}}} \quad (\text{B.8})$$

622 or equivalently, the local deviatoric stress of matrix phase becomes:

$$\boldsymbol{s} = \mathbb{K} : \mathbb{C}^m : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha} - \langle \boldsymbol{\beta} \rangle_m) = 2 \frac{\eta}{\Delta t} (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) = 2 \frac{\eta \theta}{\Delta t} (\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}_n) \quad (\text{B.9})$$

623 Finally, from (B.7), one gets

$$\boldsymbol{\alpha} = \left( \mathbb{C}^m + \frac{2\theta\eta}{\Delta t} \mathbb{K} \right)^{-1} : \left[ \mathbb{K} : \mathbb{C}^m : \boldsymbol{\varepsilon} + \frac{2\theta\eta}{\Delta t} \tilde{\boldsymbol{\alpha}}_n \right] \quad (\text{B.10})$$

## 624 Appendix C. Effective behavior and field statistics of RVE

625 The effective potential  $\Pi_0(\bar{\boldsymbol{\varepsilon}})$  is written as

$$\Pi_0(\bar{\boldsymbol{\varepsilon}}) = \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\rho}} : \bar{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\zeta}} \quad (\text{C.1})$$

where

$$\bar{\mathbb{C}} = f^m \mathbb{C}_0^m : \mathbb{A}^m + \sum_{r=1}^N f^{i,r} \mathbb{C}^{i,r} : \mathbb{A}^{i,r} \quad (\text{C.2a})$$

$$\bar{\boldsymbol{\rho}} = f^m \boldsymbol{\rho}_0^m : \mathbb{A}^m \quad (\text{C.2b})$$

$$\bar{\boldsymbol{\zeta}} = f^m (\boldsymbol{\zeta}_0^m + \boldsymbol{\rho}_0^m : \boldsymbol{a}^m) \quad (\text{C.2c})$$

626 The average of the local strain filed in the matrix can be related to the macroscopic strain by two strain  
627 concentration tensors  $\mathbb{A}^m, \boldsymbol{a}^m$ , i.e., (Willis, 1981)

$$\langle \boldsymbol{\varepsilon} \rangle_m = \mathbb{A}^m : \bar{\boldsymbol{\varepsilon}} + \boldsymbol{a}^m \quad (\text{C.3})$$

628 and similarly, the average of local strain filed in the  $r^{th}$  inclusion phase can also be described by:

$$\langle \boldsymbol{\varepsilon} \rangle_{i,r} = \mathbb{A}^{i,r} : \bar{\boldsymbol{\varepsilon}} + \boldsymbol{a}^{i,r} \quad (\text{C.4})$$

629 Note that the fourth-order tensors  $\mathbb{A}^m$  and  $\mathbb{A}^{i,r}$  can be identified to those computed for the composites  
630 in the purely elastic case. However, the expressions of second-order tensors  $\mathbf{a}^m$  and  $\mathbf{a}^{i,r}$  should be  
631 calculated by the volume averaging in each phase.

632 The second-order moment of strain filed  $\boldsymbol{\varepsilon}$  in the matrix phase can be obtained from the effective  
633 free energy  $\Pi_0(\bar{\boldsymbol{\varepsilon}})$  and by using the relations (Castañeda, 2002, Lahelec and Suquet, 2007b):

$$\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_m = \frac{2}{f^m} \frac{\partial \Pi_0}{\partial \mathbb{C}_0^m} \quad (\text{C.5})$$

634 Note that  $\mathbb{C}_0^m$  can be expressed by two effective moduli as  $\mathbb{C}_0^m = 3k^m \mathbb{J} + 2\mu_0^m \mathbb{K}$ . Then the deviatoric  
635 part of this second order moment gives (Huang et al., 2015, Lahelec and Suquet, 2007a)

$$\mathbb{K} :: \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_m = \frac{1}{f^m} \frac{\partial \Pi_0}{\partial \mu_0^m} \quad (\text{C.6})$$

636 In order to take advantage of the explicit expression of the tensors  $\mathbb{A}^m$ ,  $\mathbb{A}^{i,r}$ ,  $\mathbf{a}^m$  and  $\mathbf{a}^{i,r}$ , a two-phase  
637 material, one phase of elastic inclusion ( $r = N = 1$ ) and another phase of elastic-plastic matrix, is con-  
638 sidered for validation and application. In this case, the fourth order concentration tensors associated  
639 to the Hashin-Shtrikman (HS) estimates are adopted (Hashin, 1962)

$$\mathbb{A}^m = \mathbb{I} + \frac{1}{f^m} (\mathbb{C}_0^m - \mathbb{C}^{i,r})^{-T} : (\bar{\mathbb{C}} - \langle \mathbb{C} \rangle)^T \quad (\text{C.7a})$$

$$\mathbb{A}^{i,r} = \mathbb{I} + \frac{1}{f^{i,r}} (\mathbb{C}^{i,r} - \mathbb{C}_0^m)^{-T} : (\bar{\mathbb{C}} - \langle \mathbb{C} \rangle)^T \quad (\text{C.7b})$$

$$\mathbf{a}^m = (\mathbb{C}_0^m - \mathbb{C}^{i,r})^{-1} : (\mathbb{I} - \mathbb{A}_m)^T : \boldsymbol{\rho}_0^m \quad (\text{C.7c})$$

$$\mathbf{a}^{i,r} = -(\mathbb{C}^{i,r} - \mathbb{C}_0^m)^{-1} : (\mathbb{I} - \mathbb{A}_{i,r})^T : \boldsymbol{\rho}_0^m \quad (\text{C.7d})$$

640 where  $\langle \mathbb{C} \rangle = f^m \mathbb{C}_0^m + f^{i,r} \mathbb{C}^{i,r}$ .

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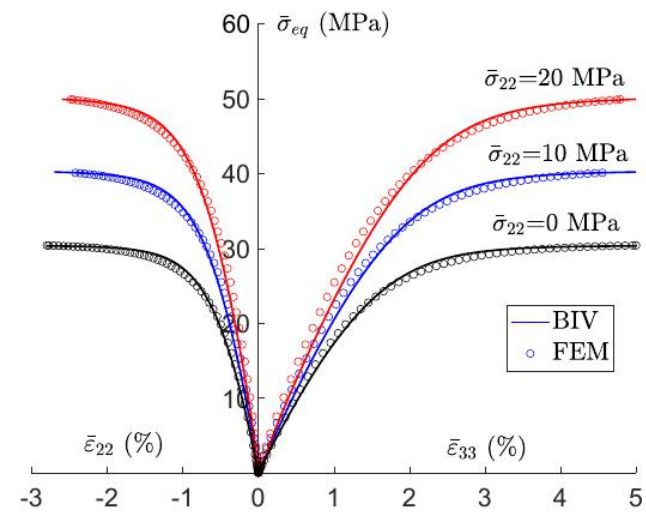
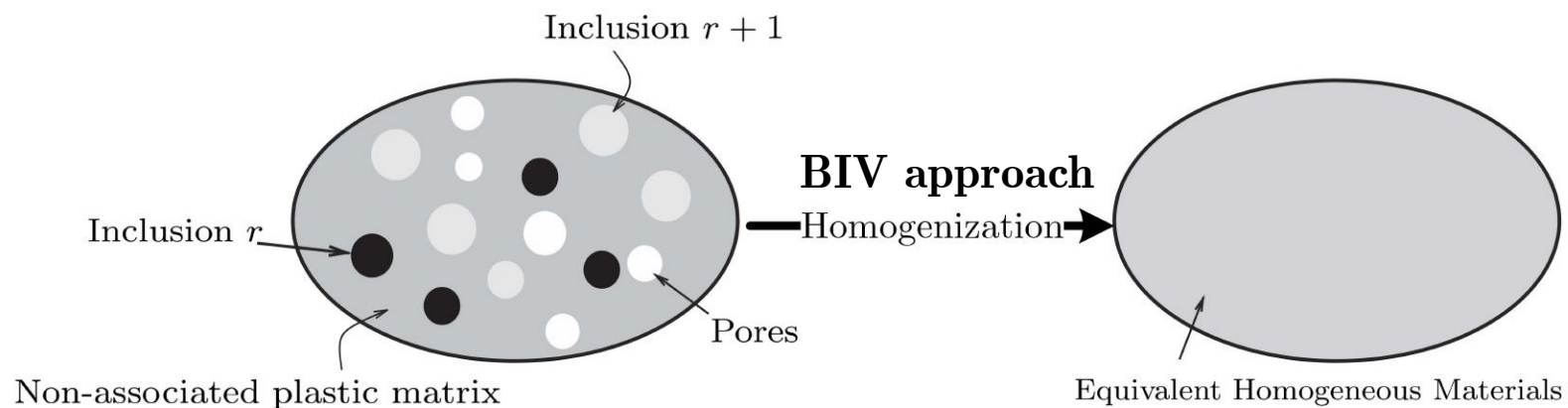
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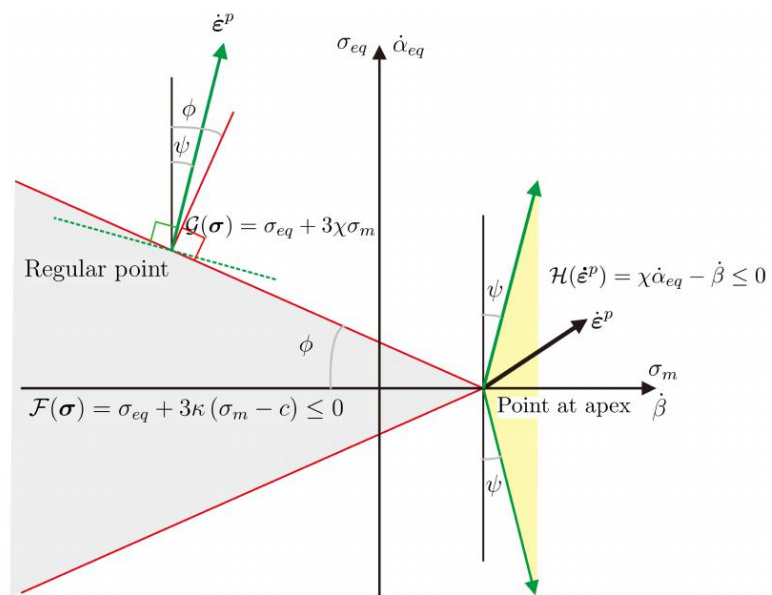
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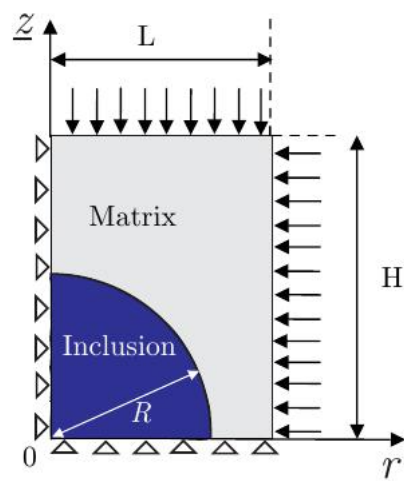
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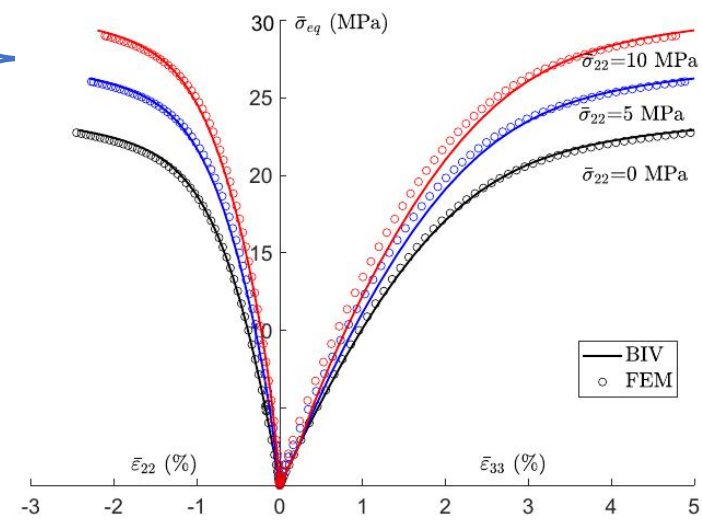
**Hard inclusion**



Drucker-Prager yield surface and non-associated plastic flow rule



Unit cell FEM simulation



**Soft inclusion**