

Journal of
Mechanics of
Materials and Structures

**A THERMOMECHANICAL FRAMEWORK OF PLASTICITY BASED
ON PROBABILISTIC MICROMECHANICS**

Itai Einav and Ian F. Collins

Volume 3, N° 5

May 2008

A THERMOMECHANICAL FRAMEWORK OF PLASTICITY BASED ON PROBABILISTIC MICROMECHANICS

ITAI EINAV AND IAN F. COLLINS

A conventional thermomechanical elasto-plastic constitutive modelling framework is proposed but which allows an effective physical interpretation of the micromechanical internal variables and inherent parameters in a representative volume element (RVE). The statistical distribution of the elastic-plastic parameters within the RVE is described using a simple statistical method of probabilistic rearrangement (MPR). This method facilitates deriving analytical approximating formulas to the stress-strain response of the RVE under unidirectional monotonic loading conditions. The applicability of the MPR is validated numerically by comparing the analytical formulas against numerical experiments of a probabilistic boundary value problem initially under monotonic conditions. The assumptions associated with the MPR are embedded within the simple micro thermomechanical constitutive framework and further evaluated numerically by applying the methodology for the case of cyclic loads. For the limited experimental program the constitutive modelling framework seems to give a rather effective estimation of the full boundary value problem. The results for the cyclic case demonstrate how hysteresis behaviour of materials could be modelled without incorporating kinematic hardening parameters.

1. Introduction

The physical properties of most solid materials in nature are spatially randomly distributed. While in some materials the randomness is given by a weak noise from the mean average, the coefficient of variance of many other materials is high. This paper will focus on modelling the class of randomly distributed heterogeneous materials, such as soils and bones, in which their micro subelements could be well described using the concepts of elasto-plasticity. Various other methods have been used to describe these materials, but the theories that are established based on physical arguments are arguably more attractive. During the years three of such continuum mechanics frameworks have been developed based on thermomechanics and micromechanics.

A first approach is to formulate the constitutive behaviour of elasto-plastic solid materials based on thermomechanics. For that purpose the class of the theories with internal variables have been described in the past including the theories of Maugin [1992] and Ulm and Coussy [2003]. Further examples follow the thermomechanical approach of Ziegler [1977], Collins and Houlsby [1997], Houlsby and Puzrin [2000], and Einav [2002]. The models of this approach are entirely derived from an explicit definition of only two potentials: energy and rate of dissipation. It is worth mentioning that there are other theories which do not use a dissipation potential [Rice 1971]. The thermomechanical frameworks provide a systematic way to describe the physical processes behind the behaviour of constitutive elements. This advantage was utilized before, based on the hyperplasticity framework, to explain the

Keywords: micromechanics, thermomechanics, constitutive modelling, plasticity, probability, kinematic hardening.

different microphysical aspects in the behaviour of granular materials [Collins and Kelly 2002; Collins and Hilder 2002; Collins and Muhunthan 2003]. In particular, the bimodal model of Collins [2005a; 2005b] provides realization based on some micromechanical interpretation. In this thermomechanical approach one actually adopts a single stress tensor and a single strain tensor to qualitatively describe the deformation within a RVE. More realistically, however, within the RVE there are variations between the local values of the microstrain and microstress tensors.

A second approach is to base the mesodomain continuum mechanics constitutive relations on the micromechanics interrelations between the microelements (or subelements). Then some form of homogenisation technique is often employed to link between the micromechanical quantities and the mesodomain RVE averaged properties [Suquet 1987; Maugin 1992; Doghri 2000]. In highly heterogeneous materials homogenisation may often lead to oversmoothing effects that are triggered by high gradients or even irregularities within the RVE. For that purpose higher order homogenisation estimates have been introduced, but they are usually developed for elastic materials [Ponte Castañeda 1996]. Such an approach was also employed to study granular materials via the use of the stored free energy [Pasternak and Mühlhaus 2005 and references cited herein]. The possibility of having frictional sliding between the grains in granular materials requires us to consider an additional potential in the form of the rate of dissipation. It is thus necessary to extend the study beyond elasticity as developed for granular materials by Vardoulakis [1983] and Chang and Ma [1991]. The main problems of this approach are that for plastic materials the existing solutions do not normally provide engineering constitutive models that can account for any loading conditions and the existing form of homogenisation either smear or fully lose the inherent memory properties of the plastic materials.

A third approach, which has recently motivated several researchers, is to combine the previous approaches in a kind of micro thermomechanics framework. Chaboche [2003] has recently proposed such a theory for elasto-plastic heterogeneous materials but was not concerned with the random aspects of the property distributions. Further examples include the works of Gurtin [2000] who has studied the constitutive behaviour of crystals, and Walsh and Tordesillas [2004] and Tordesillas et al. [2004], who have dealt with the problem of granular materials.

This paper follows the third approach dealing with a (rather large) set of problems that includes ergodic materials in which their mesodomain contains a spatially random distribution of elasto-plastic subelements [Ostoja-Starzewski 2002]. The stochastic nature of these problems is often treated numerically by assigning a particular spatial distribution of the properties in a boundary value simulation and solving this as a representative problem (see a recent review of the methods by Ostoja-Starzewski [2005]). In this way the deterministic problem carries over to the stochastic one. A second approach is to formulate the effective continuum media directly based on the governing statistics of the stochastic material [Frantziskonis 1998]. The main challenge in these works was to find analytical solutions for particular loading conditions either in the form of theoretical bounds or closed form solutions. The general statistical description of elastic-plastic media could be entirely described via an infinite set of probability functions and spatial correlation functions [Adams et al. 1989]. Approximate analytical solutions were obtained for the limiting case of a two-phase medium using the two-point probability distribution function via the correlation length [Garmestani et al. 1988]. A wider set of problems includes the infinite-phase mediums. If those phases are correlated, one has to adopt a conceptual infinite-point probability distribution function. However, when the material tends to be ergodic (and the correlation

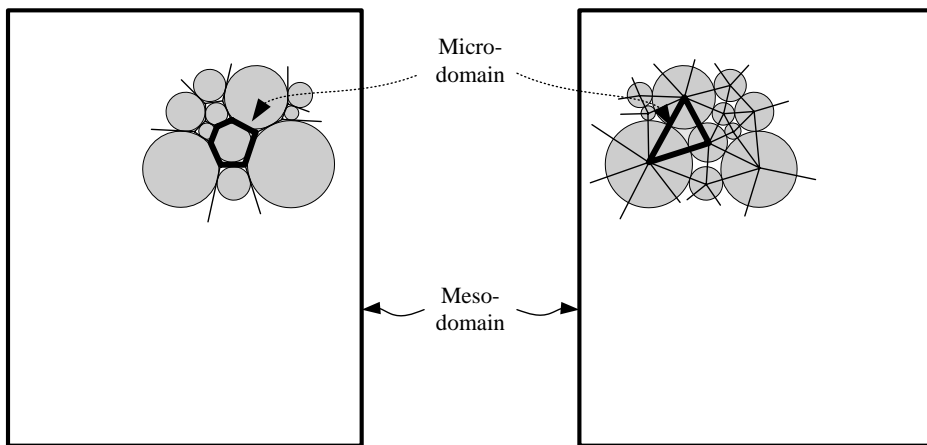


Figure 1. Definition of mesodomain and microdomain using optional tessellations (modified Voronoi or Delaunay) for the granular materials.

length becomes essentially zero), it is possible to adopt an alternative approach which we explore in this paper.

The above works, however, were mainly demonstrated for cases in which monotonic unidirectional external loads are applied to the boundaries of the RVE. The question of how to take into account cyclic events was not treated in effective manner. This paper demonstrates one possible methodology in which this could be accounted for by enabling to capture memory features that are inherent in plastic material. In particular, we find that hysteresis behaviour of random elastic-plastic materials could be attributed directly to heterogeneities without adding any *kinematic hardening parameters*. The constitutive modeling framework is also wide enough to allow estimations when the applied loads change directions.

2. Micro meso probabilistic approach

Consider a RVE that contains a collection of separate elasto-plastic subelements. Also consider materials where their microscale subelements geometries could be tessellated. For example, Figure 1 shows two optional tessellations for granular medium, discussed with other options by Satake [1978]. Due to the random physical properties of the subelements and their random geometrical configuration within the tessellation yielding occurs gradually within the RVE and this is often ignored.

Because the geometry within the RVE of a random material may be quite complicated, no attempt is made at computing the exact evolution of the micromechanics variate. Instead the goal should be to obtain estimates in terms of point statistics of the microstructure. Behind the concept of the RVE there are at least three length scales denoting the average sizes of the microscale subelements l , the mesoscale RVE size L to which the constitutive model refers to, which should be less than the macroscale size L_{macro} that corresponds to the macroscopic body size. While in the conventional homogenisation methods the averaging equation is normally additional to the constitutive equations, in the current method (which will allow creation of general constitutive models) this equation is not employed though it will be used to help in expressing the physical meaning of variables. The general average formula for general heterogeneous

problems of a variate $\hat{\bullet} = \bullet(x)$ (being the function of position x) is given by

$$\langle \hat{\bullet} \rangle = \frac{1}{V} \sum_{i=1}^N \bullet_i(x) \Delta v_i(x), \quad (1)$$

where V denotes the total volume of the RVE; i is an index counted over N homogeneous micro-subelement phases with a subvolume $\Delta v_i(x)$. The smaller length scale could be approximated by using $l \cong \sqrt[3]{\langle \Delta \hat{v} \rangle}$ and the mesolength scale by $L \cong \sqrt[3]{V}$.

Assume that $\delta = L/l \rightarrow \infty$, $L \ll L_{\text{macro}}$, and $\Delta v_i(x) = dv = l^3$ for any i , then

$$\langle \hat{\bullet} \rangle = \frac{1}{V} \int_{\text{RVE}} \bullet(x) dv. \quad (2)$$

If we further denote the use of the normalised coordinate h such that $dh = \frac{1}{v} dv = (l/L)^3$, then the length scales become nondimensional and we can integrate over a statistical volume element (SVE) [Ostoja-Starzewski 2002] from 0 to 1 rather than over the RVE

$$\langle \hat{\bullet} \rangle = \int_0^1 \bullet(h) dh. \quad (3)$$

In the above lines the hat sign over the variate $\hat{\bullet}$ was used to denote if the specific coordinate system is irrelevant, that is, $\hat{\bullet}$ could stand for both $\hat{\bullet} = \bullet(x)$ or $\hat{\bullet} = \bullet(h)$, such that $\langle \hat{\bullet} \rangle$ designates the average of the variate regardless of the coordinate system and regardless of the use of RVE (or SVE).

Methodology. Our first motivation is to set up a thermomechanical elasto-plastic framework that enables the definition of constitutive models that are complete in the classical engineering sense of providing estimates to the material response under most general loading conditions (cyclic and multidirectional). Our second motivation is to be able to deduce some micromechanical physical interpretation to the field variables and parameters. Current theories are barely achieving both tasks simultaneously. The models are either limited to monotonic unidirectional loads or they are incapable of providing a clear micromechanical interpretation. Due to the complexity of the problem this work will be based on some relaxing assumptions but in a way that allows addressing both aims.

Method of probabilistic rearrangement (MPR). In randomly distributed materials it is simply impossible to measure the physical location of all the subelements or/and their physical quantities. Thus for ergodic materials where internal geometric patterning is not present, the probability of any subelement variate in the RVE is similar to that of any other subelement. This means that the modelling of such materials may not prefer any arrangement of subelements throughout the RVE over the other and should take into account the location independency. Therefore, for example in granular materials, a change in position of two particles in infinite assembly (as represented schematically in Figure 2) should not affect the structure of the constitutive models, since we have no means to distinguish one arrangement as being practically better than the other. This is a rather different approach to take deterministically a particular spatial configuration and carry out computations based on it.

Assume that the micromechanical variates (such as the strength and stiffness coefficients) are constant in each of the subelements but randomly distributed throughout the RVE. The volume that each subelement captures could be denoted as Δv_i . The values of a particular variate could be arranged in a

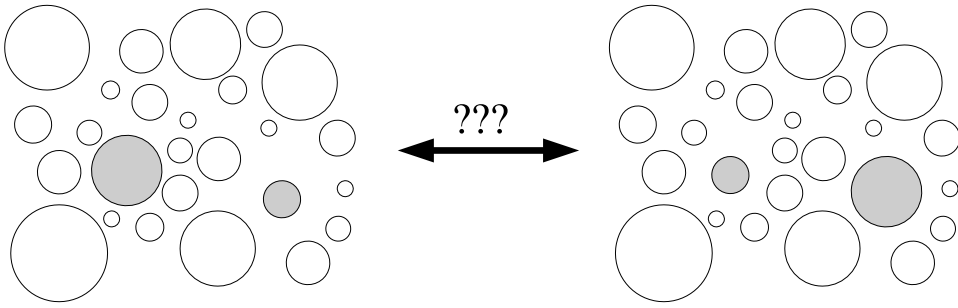


Figure 2. The enigma of what is the right deterministic representation: any discrete particle configuration is possible from a mesoscopic point of view thus none of them could be viewed as better when formulating *engineering* continuum models.

line according to its spatial physical volume coordinate order x , and since the micromechanics quantity is assumed constant within each subelement, its variation throughout the entire RVE with the index i may be schematically described by Figure 3a. Since any optional deterministic spatial arrangement of subelements may not be viewed as better than the others, the chaotic distribution of Figure 3a could be rearranged in a monotonic order as in Figure 3b.

When the number of elements in the RVE is essentially infinite, the discrete plot can be effectively replaced by a continuous distribution function denoting the changes of the micromechanics quantity over the rearranged normalised volume coordinate h in a SVE. We identify a statistical physical meaning to the coordinate $h \equiv p$ as the significance cumulative probability of the system. The distribution function of the micromechanics quantity is identified as the percent point function or the inverse cumulative distribution function (inverse cdf), as it returns the critical values of the micromechanics variate for hypothesis testing

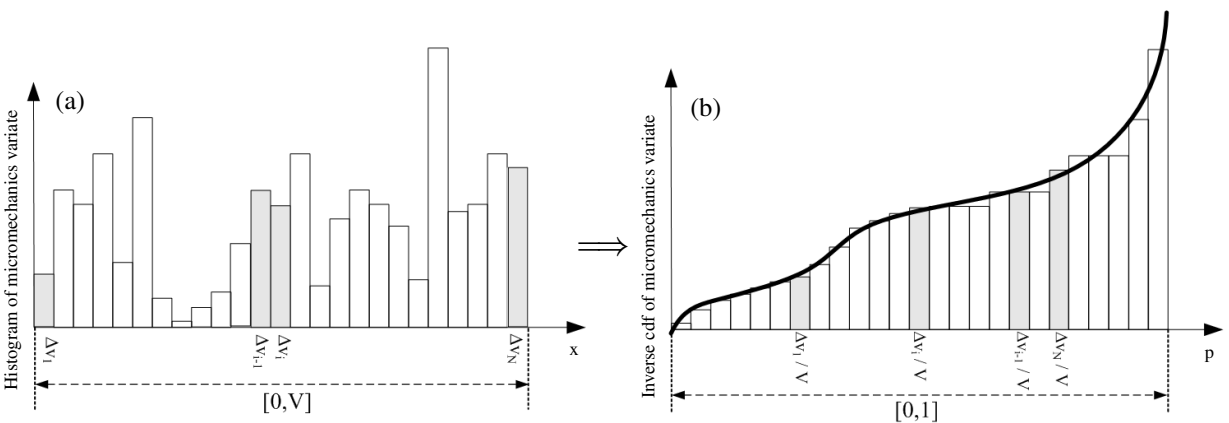


Figure 3. Method of probabilistic rearrangement (a) Histogram of a micromechanics along physical volume coordinate x in the RVE, and (b) Inverse cumulative distribution along the rearranged relative volume p (being the cumulative probability).

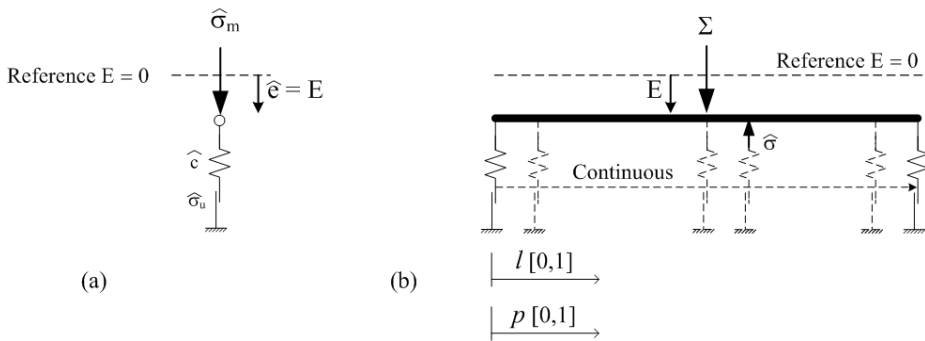


Figure 4. The construction of conceptual micro thermomechanical one-dimensional plasticity model: (a) St-Venant model. (b) continuous Masing-Iwan model (after [Einav 2005]).

given significance cumulative probabilities. Therefore Equation (3) could be rewritten

$$\langle \hat{\bullet} \rangle = \int_0^1 \bullet(p) dp$$

while the integration from zero to one is activated over the entire cumulative probability space.

3. Conceptual one-dimensional micro thermomechanical plasticity model

Let us start with the one-directional model proposed by Einav [2005] as an extension to the discrete Masing-Iwan model. The model is built on a continuous parallel system of pointwise St-Venant spring-slider elements (see Figure 4 for the description of an individual St-Venant element and the complete continuous Masing-Iwan system). The mechanical/structural properties of this model are reinterpreted based on the probabilistic approach. The model provides motivation and serves as a simple introduction towards the formalism which is being derived in the next section.

3.1. Interlinks between mechanical and probabilistic concepts. All of the “legs” in the continuous Masing-Iwan system undergo the same total scalar strain E . The model is initially dependent on two stochastic distributions $\sigma_u(x)$ and $c(x)$ denoting the slider threshold and elastic stiffness coefficients along the physical spatial volume coordinate $x \in [0, V]$. Using MPR the previous distribution function may also be expressed based on the probability coordinate $p \in [0, 1]$: $\sigma_u(p)$ and $c(p)$. Further suppose that $\sigma_u(p)$ is a monotonically increasing function and that $c(p)$ is smooth. The distribution $\sigma_u(p)$ is interpreted as the inverse cdf returning the value of significant plastic threshold $\sigma_u(p_a)$ for a given cumulative probability $p = p_a$. $c(p)$ is identified as the distribution of the microscale elastic moduli along the plastic threshold cumulative probability p .

To designate the interchangeable nature of the original system ($\sigma_u(x)$ and $c(x)$) and the rearranged system ($\sigma_u(p)$ and $c(p)$), we shall use the hat sign over the variates and remove the coordinate, that is, $\hat{\sigma}_u$ and \hat{c} will denote the microscale slider threshold and elastic stiffness coefficients regardless of the coordinate. This designation method is used throughout the text.

If $\hat{\sigma}$ denotes the microstress within a corresponding St-Venant element (Figure 4a) then from equilibrium the total stress Σ (not to be mistaken with the summation sign) is given by

$$\Sigma = \frac{1}{V} \int_0^V \sigma(x) dx = \int_0^1 \sigma(p) dp = \langle \hat{\sigma} \rangle$$

such that it is observed that Σ also equals the average over the microscale stresses $\hat{\sigma}$ within the RVE using Equation (2) or within the SVE using Equation (3). Furthermore it is noted that equilibrium in the mechanical system has nothing to do with the order of the St-Venant constituents thus demonstrating that the MPR is valid whenever strains are uniform throughout the RVE.

The microstress is linearly related to the microelastic strain within the micro Saint-Venant element. In the original system this is expressed by

$$\sigma(x) = c(x)(E - e_p(x)) = c(x) e_e(x),$$

where E is the mesostrain and is uniform in this model, that is, $E = e(x)$ for any x ; $e(x)$, $e_e(x)$, and $e_p(x)$ denote the total, elastic, and plastic microstrains at the spatial coordinate x .

In the rearranged system this may be expressed by

$$\sigma(p) = c(p)(E - e_p(p)) = c(p) e_e(p), \quad (4)$$

where $e_e(p)$ and $e_p(p)$ are now functions of the cumulative probability p .

3.2. Thermomechanical potentials. The Helmholtz free energy density at the x spatial coordinate or the p probability coordinate of the microscale spring are given by

$$\begin{aligned} \hat{\psi} &= \psi(E, e_p(x), x) = \frac{c(x)}{2} e_e(x)^2 = \frac{c(x)}{2} (E - e_p(x))^2, \\ \hat{\psi} &= \psi(E, e_p(p), p) = \frac{c(p)}{2} e_e(p)^2 = \frac{c(p)}{2} (E - e_p(p))^2. \end{aligned}$$

Both could be integrated to give the total Helmholtz free energy functional of the system

$$\Psi(E, \hat{e}_p) = \frac{1}{V} \int_{\text{RVE}} \frac{c(x)}{2} (E - e_p(x))^2 dx = \int_0^1 \frac{c(p)}{2} (E - e_p(p))^2 dp = \langle \hat{\psi} \rangle. \quad (5)$$

It is shown how the total Helmholtz free energy functional agrees with the average of the local potential densities within the RVE.

The rate of local rate of dissipation density associated with the microscale slider in the x spatial coordinate or the p probability coordinate is given by¹

$$\hat{\phi} = \tilde{\phi}(\dot{e}_p(x), x) = \sigma_u(x) |\dot{e}_p(x)| \geq 0, \quad \hat{\phi} = \tilde{\phi}(\dot{e}_p(p), p) = \sigma_u(p) |\dot{e}_p(p)| \geq 0. \quad (6)$$

¹We are using a “tilde” instead of the more usual “dot” notation for the time derivative, to emphasize that there is no state dissipation function $\hat{\phi}$.

The rate of dissipation is not a point function and it is path dependent. Integration of the rate of local dissipation density over the full domains suggests the total rate of dissipation

$$\tilde{\Phi}(\dot{\hat{e}}_p) = \frac{1}{V} \int_{RVE} \tilde{\phi}(\dot{e}_p(x), x) dx = \int_0^1 \tilde{\phi}(\dot{e}_p(p), p) dp = \langle \hat{\phi} \rangle \geq 0. \quad (7)$$

It is shown that the total rate of dissipation agrees with the average of the local potential densities within the RVE (or SVE).

Inversely, we will later demonstrate (see the first example in the example section) how the entire constitutive behaviour of the one-dimensional model is encapsulated in Equations (5) and (7).

4. Thermomechanical micro meso plasticity

In this paper we consider a mesocontinuum system which is composed from an infinite field of infinitesimal microcontinua. Each of the microcontinua is described by an elasto-plastic model with a single plastic internal variable, such that the description of the mesocontinuum is given by a set of infinite field of plastic internal variables (or a plastic internal function of the corresponding coordinate). The first and second laws of thermodynamics of the constitutive behaviour of rate independent isothermal materials should hold in both microform (local) and mesoform (global).

In *microform* the laws are given by the expression

$$\tilde{w} = \dot{\hat{\psi}} + \hat{\phi}, \quad \hat{\phi} \geq 0, \quad (8)$$

where $\hat{\psi}$ is the (micro) Helmholtz free energy density, $\hat{\phi}$ is the (micro) rate of energy dissipation density (which has to be nonnegative), and $\tilde{w} = \hat{\sigma} : \dot{\hat{e}}$ denotes the rate of the mechanical work done on the microcontinuum element, all defined per unit volume; finally the symbol ‘:’ denotes the inner product of two tensors. The notations of the scalar microstress $\hat{\sigma}$ and microstrain \hat{e} from the previous sections are changed by the bold face, denoting the more general case of second order tensors $\hat{\sigma}$ and \hat{e} . As stated before the Helmholtz free energy density is assumed to be a function of state unlike the rate of dissipation density and mechanical work density.

In *mesoform* the laws are given by the expression

$$\tilde{W} = \dot{\Psi} + \tilde{\Phi}, \quad \tilde{\Phi} \geq 0, \quad (9)$$

where Ψ is the (meso) Helmholtz free energy, $\tilde{\Phi}$ is the nonnegative (meso) rate of energy dissipation and

$$\tilde{W} = \Sigma : \dot{E}$$

denotes the rate of the mechanical work done on the boundaries of the mesocontinuum element, all defined per unit volume.

As the laws of thermodynamics should hold anywhere within the RVE, an alternative mesoform of the laws of thermodynamics could be given simply by up-scaling or integrating Equation (8) over the RVE (or the SVE)

$$\langle \tilde{w} \rangle = \langle \dot{\hat{\psi}} \rangle + \langle \hat{\phi} \rangle, \quad \langle \hat{\phi} \rangle \geq 0. \quad (10)$$

By identifying the additivity of internal energy and rate of dissipation $\Psi = \langle \hat{\psi} \rangle$ and $\tilde{\Phi} = \langle \hat{\phi} \rangle \geq 0$, while for a statically admissible stress field and a kinematically admissible displacement field [Hill 1963; Suquet

1987; Maugin 1992], the classical Hill-Mandel equality could be found

$$\Sigma : \dot{\mathbf{E}} = \langle \hat{\sigma} : \hat{\dot{\mathbf{e}}} \rangle. \tag{11}$$

The procedure, which relates Σ and \mathbf{E} (and possibly their derivatives with respect to the time and other parameters) by means of Equations (8) and (9) and the micro constitutive laws, is termed *homogenisation*. The inverse, termed *localization*, amounts to a micromechanics problem which permits determining microscopic quantities as $\hat{\sigma}$ and $\hat{\mathbf{e}}$. For ergodic material, the RVE (or SVE) has a large size with respect of the heterogeneity's size, so that the "stress vector" $\sigma(x) \cdot \mathbf{n}(x)$ or the displacement vector $u(x)$ on the boundaries fluctuate about a mean with a small wavelength compared with the dimensions of the RVE. In this case, the boundary stress and strain tensors are equal to the average of the stress and strain field tensors within the RVE.

A localisation analysis is suggested to identify the constitutive relations at the microlevel followed by homogenisation analysis to determine the quantities at the mesolevel.

4.1. Localisation analysis (microrelations). For the micro constitutive problem the micro Helmholtz free energy density is given directly as the free energy of elasto-plastic models

$$\hat{\psi} = \hat{\psi}_1(\hat{\mathbf{e}} - \hat{\mathbf{e}}_p) + \hat{\psi}_2(\hat{\mathbf{e}}_p) = \hat{\psi}_1(\hat{\mathbf{e}}_e) + \hat{\psi}_2(\hat{\mathbf{e}}_p), \tag{12}$$

where $\hat{\mathbf{e}}_e$ and $\hat{\mathbf{e}}_p$ are the microelastic and plastic strains, satisfying $\hat{\mathbf{e}} = \hat{\mathbf{e}}_e + \hat{\mathbf{e}}_p$. The first component in Equation (12), $\hat{\psi}_1(\hat{\mathbf{e}}_e)$, is related to the "stored energy" in the system and is linked with the elasticity law, while the second term $\hat{\psi}_2(\hat{\mathbf{e}}_p)$ is referred to as the "frozen energy" [Ulm and Coussy 2003; Collins 2005b]. In the following we ignore the possibility of frozen energy in the microscopic level and specialize the micro free energy density by

$$\hat{\psi} = \hat{\psi}_1(\hat{\mathbf{e}} - \hat{\mathbf{e}}_p) = \hat{\psi}_1(\hat{\mathbf{e}}_e). \tag{13}$$

In the case of rate-independent processes of elasto-plastic models the rate of the dissipation function is a homogeneous first order function of the plastic strain rate. This homogeneity can be expressed by Euler's equation

$$\hat{\hat{\phi}}(\hat{\mathbf{e}}, \hat{\mathbf{e}}_p, \dot{\hat{\mathbf{e}}}_p) = \frac{\partial \hat{\hat{\phi}}}{\partial \dot{\hat{\mathbf{e}}}_p} : \dot{\hat{\mathbf{e}}}_p \geq 0. \tag{14}$$

Combining the last two equations with Equation (8) gives the micro generalized (dissipative) stress and Cauchy stress tensors

$$\begin{aligned} \hat{\sigma} &= \frac{\partial \hat{\psi}(\hat{\mathbf{e}}, \hat{\mathbf{e}}_p)}{\partial \hat{\mathbf{e}}} = \frac{\partial \hat{\psi}_1(\hat{\mathbf{e}} - \hat{\mathbf{e}}_p)}{\partial \hat{\mathbf{e}}} = \hat{\psi}'_1(\hat{\mathbf{e}}_e) \\ \hat{\chi} &= -\frac{\partial \hat{\psi}_1(\hat{\mathbf{e}} - \hat{\mathbf{e}}_p)}{\partial \hat{\mathbf{e}}_p} = \hat{\psi}'_1(\hat{\mathbf{e}}_e) \quad \left(= \frac{\partial \hat{\hat{\phi}}}{\partial \dot{\hat{\mathbf{e}}}_p}, \text{ whenever } \dot{\hat{\mathbf{e}}}_p \neq 0 \right). \end{aligned} \tag{15}$$

The equality in the brackets of Equation (15) agrees with Ziegler's orthogonality condition. In the particular form of Equation (13) we find that the micro generalized stress $\hat{\chi}$ is actually the micro Cauchy stress

$$\hat{\chi} = \hat{\sigma}. \tag{16}$$

Each rate of micro dissipation density could be linked to a single micro yield surface using degenerate Legendre transformation

$$\hat{\lambda} \hat{y}(\hat{\boldsymbol{e}}, \hat{\boldsymbol{e}}_p, \hat{\chi}) = \hat{\phi}(\hat{\boldsymbol{e}}, \hat{\boldsymbol{e}}_p, \dot{\hat{\boldsymbol{e}}}_p) - \hat{\chi} : \dot{\hat{\boldsymbol{e}}}_p \equiv 0. \quad (17)$$

The conventional shift stress term $\hat{\psi}'_2(\hat{\boldsymbol{e}}_p)$ is not added to the micro generalized stress $\hat{\chi}$ expression (16) because of the assumption $\hat{\psi}_2 = 0$. This means that in microscopic terms yield surfaces do not translate in the stress space [Houlsby and Puzrin 2000]. In other words, in this case kinematic hardening in the microlevel is taken out of consideration (although models could still harden in the isotropic hardening sense). In kinematic hardening plasticity or other plasticity variants kinematic hardening parameters are often added within the terms $\hat{\psi}_2(\hat{\boldsymbol{e}}_p)$, which are omitted in the current formulation, to explain the Masing hysteretic behaviour of elasto-plastic materials. It will be shown that at the mesoscopic scale, however, the Masing hysteresis could still be deduced without introducing the $\hat{\psi}_2(\hat{\boldsymbol{e}}_p)$ terms (in other words without including kinematic hardening parameters at the microscopic level).

4.2. Homogenisation analysis (mesorelations). The previous subsection detailed the derivation of the microelasto-plastic constitutive relations between the micro stresses $\hat{\boldsymbol{\sigma}}$ and strains $\hat{\boldsymbol{e}}$ from the definition of micro rate of dissipation and free energy density functions. This section describes the derivation of the mesoscopic relation from the meso Helmholtz free energy and rate of dissipation potentials. For the random elasto-plastic problem these are given by integrating the micropotentials over the RVE (or SVE) with Equations (9), (10), (13) and (14)

$$\Psi = \langle \hat{\psi}_1(\hat{\boldsymbol{e}}_e) \rangle = \langle \hat{\psi}_1(\hat{\boldsymbol{e}} - \hat{\boldsymbol{e}}_p) \rangle, \quad \tilde{\Phi} = \langle \hat{\phi}(\hat{\boldsymbol{e}}, \hat{\boldsymbol{e}}_p, \dot{\hat{\boldsymbol{e}}}_p) \rangle. \quad (18)$$

The mesoscopic relations represent a boundary value problem that links between the internal microscale field variables and the mesoscopic boundary variables Σ and \boldsymbol{E} ideally taking into account microstress equilibrium and compatibility relations while satisfying the Hill-Mandel work equilibrium in Equation (11). For simple problems, such as linear elastic heterogeneous problems, it is then possible to derive closed form solutions [Suquet 1987]. As our problem is much more involved than the linear elastic problem, and the focus is equally given to derive a conventional framework of elasto-plasticity, we take the assumption of uniform strain assuming that the microscale strain is uniform throughout the RVE. The fact that the total strain is the same for all subelements is equivalent to the Voigt homogenisation scheme. A more general analysis would have a different total strain for each subelement. The result is that equilibrium is satisfied only in the weak (Hill-Mandel) work form. In elastic materials the uniform strain assumption is known to provide an upper bound to the overall stiffness of the system, while the alternative assumption of uniform stress would provide a lower bound [Doghri 2000]. The more advanced theories for such materials may in fact narrow the distance between the bounds and may thus offer more predictive models. However, we are concerned with elasto-plastic models. Defining elasto-plasticity models using the more advanced hypotheses would lead to rather more complicated equations that we tend to avoid at this early stage. Between the two simple equivalence hypotheses, the uniform strain and uniform stress, the first is more often used [Walton 1987; Vardoulakis and Sulem 1995; Houlsby and Sharma 1999] as stresses are much more heterogeneous as is evidenced from experiments [Drescher and de Josselin de Jong 1972] or from looking at DEM simulations [Cundall and Strack 1979]. The uniform strain assumption suggests that $\hat{\boldsymbol{e}} = \boldsymbol{E}$ for any coordinate x or p . Therefore since the strains

(and strain rates) are essentially deterministic, the statement $\dot{\mathbf{E}} = \langle \dot{\hat{\mathbf{e}}} \rangle = \dot{\hat{\mathbf{e}}}$ is trivial and not a result of statistical averaging. On the other hand, the macrolevel stress is a result of ensemble averaging satisfying the Hill-Mandel relation (11) with

$$\Sigma = \langle \hat{\sigma} \rangle = \langle \hat{\psi}'_1(\hat{\mathbf{e}}_e) \rangle. \quad (19)$$

The strain decomposition is thus given by

$$\mathbf{E} = \hat{\mathbf{e}}_e + \hat{\mathbf{e}}_p, \quad (20)$$

where we note that while the strain is uniform, the elastic and plastic strains are not. In this case the potentials could be specialized by

$$\Psi = \langle \hat{\psi}_1(\mathbf{E} - \hat{\mathbf{e}}_p) \rangle, \quad \tilde{\Phi} = \langle \hat{\phi}(\mathbf{E}, \hat{\mathbf{e}}_p, \dot{\hat{\mathbf{e}}}_p) \rangle. \quad (21)$$

The relations between the above and the simple motivating springs-sliders model example in Equations (5), (7) are apparent. The transformation to the field of yield surfaces (17) is then

$$\hat{\lambda} \hat{y}(\mathbf{E}, \hat{\mathbf{e}}_p, \hat{\chi}) = \hat{\phi}(\mathbf{E}, \hat{\mathbf{e}}_p, \dot{\hat{\mathbf{e}}}_p) - \hat{\chi} : \dot{\hat{\mathbf{e}}}_p \equiv 0.$$

Thus

$$\dot{\hat{\mathbf{e}}}_p = \hat{\lambda} \partial \hat{y} / \partial \hat{\chi}.$$

The rate form of Equation (19) is given by

$$\dot{\Sigma} = \langle \hat{\psi}''_1(\hat{\mathbf{e}}_e) \rangle : \dot{\mathbf{E}} - \langle \hat{\psi}''_1(\hat{\mathbf{e}}_e) \rangle : \dot{\hat{\mathbf{e}}}_p.$$

The global instantaneous elastic stiffness moduli tensor could be defined when all the microscale plastic strain rates are zero

$$\mathbf{M} = \langle \hat{\psi}''_1(\hat{\mathbf{e}}_e) \rangle, \quad (22)$$

such that it is found that the elastic stiffness is a function of the microscale elastic strains. This means that the instantaneous modulus is not constant upon unloading-reloading, and is dependent upon the stored elastic energy.

The mesopotentials (21) are functionals of internal plastic strain tensor variable $\hat{\mathbf{e}}_p$ of either the x or p internal coordinates, while any yield surface in the field is associated with a given coordinate. The concept of incorporating an internal variable tensor function $\alpha(\eta)$ of some internal coordinate η and defining a continuous field of yield surfaces in a thermomechanically admissible framework was recently introduced by Puzrin and Houlsby [2001]. But the defined class of potentials $\alpha(\eta)$ and η did not receive any significant physical meaning. Masing hystereses were modelled via a separate kinematic hardening distribution function of η , and models were based on curve fitting this distribution function to experimental laboratory data [Puzrin et al. 2001; Einav and Puzrin 2004]. Here Masing hystereses are obtained without including an additional kinematic hardening distribution function.

The above form of the Helmholtz free energy potential functional was proposed independently by Chaboche [2003] and Einav [2005] though in the first case in a more limited form allowing only for linear elasticity (assuming quadratic free energy functions). A more significant change is that the treatment of the derivation is completely different. Chaboche [2003] explored the outcomes of employing these functionals using traditional homogenization techniques seeking to replace the set of plastic internal

variables using a single plastic variable, but here we will adopt the MPR that enables us to keep track of the entire field of plastic internal variables. This, in turn, allows deriving a more detailed set of evolution equations without loosing memory aspects of plastic materials. Also, the result is that a field of yield surfaces in the micro stress space is defined rather than a single yield surface as Chaboche [2003] suggested.

4.3. Micro thermomechanics with linear microelasticity. Equation (18) (left) could be specialized by limiting its form to linear microelasticity, by suggesting a general homogeneous function of degree 2 of the microscale elastic strains

$$\Psi = \frac{1}{2} \langle \hat{\mathbf{e}}_e : \hat{\mathbf{m}} : \hat{\mathbf{e}}_e \rangle, \quad \text{that is} \quad \hat{\psi}_1(\hat{\mathbf{e}}_e) = \frac{1}{2} \hat{\mathbf{e}}_e : \hat{\mathbf{m}} : \hat{\mathbf{e}}_e, \quad (23)$$

where $\hat{\mathbf{m}}$ is a fourth order tensor function denoting the variation in microscale elastic stiffness coefficients within the RVE; this function is chaotic with the spatial coordinate x but assumed to be smooth with the cumulative probability p . Based on Equations (19) and (20) the stress is given by

$$\Sigma = \langle \hat{\mathbf{m}} \rangle : \mathbf{E} - \langle \hat{\mathbf{m}} : \hat{\mathbf{e}}_p \rangle,$$

which upon further derivation gives the fourth-order mesoscale stiffness tensor

$$\mathbf{M} = \partial \Sigma / \partial \mathbf{E} = \langle \hat{\mathbf{m}} \rangle. \quad (24)$$

This equation should be compared with the elastic stiffness tensor of the general nonlinear case (22). This time this tensor is not a function of the microscale elastic strains.

4.4. A discrete approximation of models (probabilistic system). In Section 4.2 the general structure of continuous potentials were listed. Under monotonic unidirectional loading conditions, using the smooth probabilistic system, it is possible to derive closed form expressions (as will be demonstrated in the next section) describing the stress-strain curve response of the material. For general loading conditions, when the material is cyclically loaded or the direction of loading alters, it is convenient to use an alternative effective *numerical* scheme. An efficient way to do it is to approximate the general continuous potentials (given by Equation (21)) discretely

$$\Psi = \int_0^1 \psi_1(\mathbf{e}_e(p), p) dp \approx \sum_{n=1}^N \psi_1(\mathbf{e}_e(p_n), p_n) \Delta p_n = \sum_{n=1}^N \psi_1^n(\mathbf{e}_e^n),$$

$$\tilde{\Phi} = \int_0^1 \tilde{\phi}(\mathbf{E}, \mathbf{e}_p(p), \dot{\mathbf{e}}_p(p), p) dp \approx \sum_{n=1}^N \tilde{\phi}(\mathbf{E}, \mathbf{e}_p(p_n), p_n) \Delta p_n = \sum_{n=1}^N \tilde{\phi}_n(\mathbf{E}, \mathbf{e}_p^n, \dot{\mathbf{e}}_p^n),$$

where p_n denotes a particular cumulative probability point, N is the number of those points, Δp_n is a vector of length N denoting the zone of influence of each of these approximating points. The discrete approximation of the rate of dissipation leads to definition of a field of N yield surfaces rather than a continuous field

$$\tilde{\lambda}_n y_n(\mathbf{E}, \mathbf{e}_p^n, \chi_n) = \tilde{\phi}_n(\mathbf{E}, \mathbf{e}_p^n, \dot{\mathbf{e}}_p^n) - \chi_n : \dot{\mathbf{e}}_p^n \equiv 0,$$

where we note that

$$y_n(\mathbf{E}, \mathbf{e}_p^n, \chi_n) = y\left(\mathbf{E}, \mathbf{e}_p(p_n), \frac{\chi(p_n)}{\Delta p_n}, p_n\right).$$

The above allows one, following a standard computational method, to derive rather effectively the response of the continuous problem in a discrete numerical manner. As $\chi_n = \sigma_n$, the consistency condition of the n -th yield surface is given by

$$\dot{y}_n(\mathbf{E}, \mathbf{e}_p^n, \sigma_n) = \frac{\partial y_n}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial y_n}{\partial \mathbf{e}_p^n} : \dot{\mathbf{e}}_p^n + \frac{\partial y_n}{\partial \sigma_n} : \dot{\sigma}_n = 0,$$

which together with the n -th flow rule $\dot{\mathbf{e}}_p^n = \tilde{\lambda}_n \partial y_n / \partial \sigma_n$, the n -th decomposition of strains $\dot{\mathbf{E}} = \dot{\mathbf{e}}_e^n + \dot{\mathbf{e}}_p^n$, and the rate form of the microelasticity rule $\dot{\sigma}_n = \psi_1^{n''}(\mathbf{e}_e^n) : \dot{\mathbf{e}}_e^n$ gives the solution for the n -th nonnegative microplasticity multiplier

$$\tilde{\lambda}_n = \left(\frac{\frac{\partial y_n}{\partial \mathbf{E}} + \frac{\partial y_n}{\partial \sigma_n} : \psi_1^{n''}(\mathbf{e}_e^n)}{\frac{\partial y_n}{\partial \sigma_n} : \psi_1^{n''}(\mathbf{e}_e^n) : \frac{\partial y_n}{\partial \sigma_n} - \frac{\partial y_n}{\partial \mathbf{e}_p^n}} \right) : \dot{\mathbf{E}},$$

which upon elimination and the rate form of $\Sigma = \sum_{n=1}^N \sigma_n$ evolution law (note that “ Σ ” and “ \sum ” denote the meso stress tensor and the sum operator, respectively)

$$\dot{\Sigma} = \sum_{n=1}^N \psi_1^{n''}(\mathbf{e}_e^n) : \left(\dot{\mathbf{E}} - \tilde{\lambda}_n \frac{\partial y_n}{\partial \sigma_n} \right).$$

5. Examples

5.1. One-directional monotonic loading of the one-dimensional basic model. The potentials of the conceptual model in Section 3 (Equations (5) and (7)) were defined based on the mechanical role of the constituents. Then the structure of those potentials was generalised in Section 4 and we showed how the rate of global dissipation leads to a definition of a field of yield surfaces (each yield surface is associated with a corresponding rate of dissipation density). In this section we will demonstrate how stress-strain relations could be derived directly from the potentials. It is possible to examine the model performance for one-directional monotonic loading conditions. For such derivation, since the original system is chaotic, the rearranged system helps in finding analytical solutions. To this end we adopt the MPR. The local rate of dissipation density is given by Equation (6) and $\tilde{\phi}(\dot{e}_p(p), p) = \sigma_u(p) |\dot{e}_p(p)| \geq 0$. According to the Equation (15), in the rearranged system we can define the dissipative generalised stress as

$$\chi(p) = -\partial \tilde{\phi} / \partial \dot{e}_p(p) = \sigma_u(p) \operatorname{sgn}(\dot{e}_p(p)) \geq 0,$$

where $\operatorname{sgn}(\cdot)$ denotes the signum function. The presence of the rate of the microplastic strain $\dot{e}_p(p)$ could be eliminated by taking the absolute of both sides, and this defines the yield surface in the local dissipative generalized stress space

$$y(\chi(p), p) = |\chi(p)| - \sigma_u(p) \leq 0.$$

Invoking Ziegler’s orthogonality hypothesis, the dissipative stress $\chi(p)$ could also be derived from the Helmholtz free energy potential density

$$\chi(p) = -\partial \psi(E, e_p(p)) / \partial e_p(p) = \sigma(p) = c(p)(E - e_p(p))$$

and thus the sliding condition in the different St-Venant elements could be represented alternatively by yield functions in the microstress or in the mesostrain spaces

$$F(\sigma(p), p) = |\sigma(p)| - \sigma_u(p) \leq 0, \quad F(E, e_p(p), p) = |c(p)(E - e_p(p))| - \sigma_u(p) \leq 0. \quad (25)$$

The performance of the basic model is dependent on the distribution functions $\sigma_u(p)$ and $c(p)$. The strength distribution curve for ductile solids is very narrow, while that for brittle solids is very broad with a large tail on the larger-strength side that can be explained by a statistical distribution called the Weibull distribution [Weibull 1951]. Weibull statistics was used extensively to describe brittle solids such as ceramics [Espinosa and Zavattieri 2003] and is based on the principle that the survival of a block under tension requires that all its constituents parts remain intact (a chain is as strong as its weakest link). A similar understanding was recently adopted to explain the statistical crushing events in the compression of soils [McDowell and Bolton 1998; Nakata et al. 1999].

The probability density function (pdf) of the two-parameter Weibull distribution is given by $f(x) = (\beta/\alpha)(x/\alpha)^{\beta-1} \exp(-(x/\alpha)^\beta)$, for all $\{x, \alpha, \beta\} \geq 0$, where α is known as the scale parameter and β as the shape parameter. Thus the two-parameters Weibull cumulative distribution function (cdf) is given by $F(x) = P_r[X \leq x] = \int_{-\infty}^x f(\mu)d\mu = 1 - \exp(-(x/\alpha)^\beta)$. For the inverse cdf we start with the probability and compute the corresponding x for the cumulative distribution. Mathematically this can be expressed by defining the function $G(p)$ of the cumulative probability p as $P_r[X \leq G(p)] = p$, for all $p \in [0, 1]$, such that $x = G(p) = G(F(x))$. Thus for the two-parameters Weibull function the inverse cdf is $G(p) = \alpha[-\ln(1 - p)]^{1/\beta}$. Figure 5 shows the normalised Weibull inverse cdf $G(p)/\alpha$ for varying β values. It could be seen that α is the inverse cdf value that corresponds to cumulative distribution of about 67%. Normalising of the last expression by the mean value of the Weibull pdf, given by $\bar{T} = \alpha\Gamma(1 + 1/\beta)$, where $\Gamma(x) = \int_0^\infty \mu^{x-1} \exp(-\mu)d\mu$ is the Gamma function, and multiplying by Σ_u gives

$$\sigma_u(p) = \frac{\Sigma_u}{\bar{T}} G(p) = \frac{\Sigma_u[-\ln(1 - p)]^{1/\beta}}{\Gamma(1 + 1/\beta)}. \quad (26)$$

It could be checked that Σ_u is

$$\Sigma_u = \int_0^1 \sigma_u(p) dp = \langle \hat{\sigma}_u \rangle$$

such that it plays the role of a parameter that defines the mesoscale complete failure, that is, the stress at which all sliders become active, and is equal to the average of all the constituents' plastic threshold.

Contrary to the common assumption of the suitability of the Weibull distribution in describing the failure of materials, there is no apparent evidence, at least that we are aware of, suggesting such a dependency of the elastic moduli. For this reason let us assume constant elastic stiffness

$$c(p) = C_0 \quad (27)$$

suggesting uniform instantaneous elastic moduli C_0 in the SVE.

The two inverse cumulative distribution functions of Equations (26) and (27) are plotted qualitatively in Figure 6. In this figure the shaded area represents the contribution of the microstresses to balance the applied mesostress. Mathematically this could be expressed

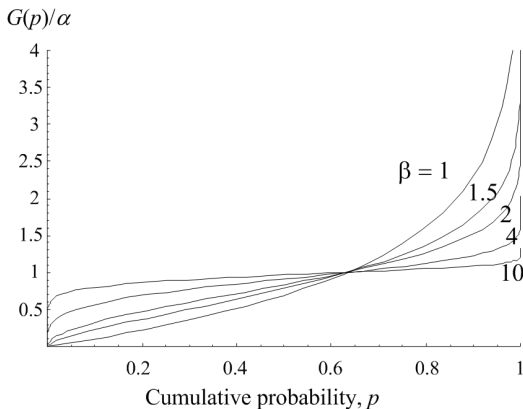


Figure 5. Normalized inverse cdf for different shape parameter β of the Weibull distribution.

$$\begin{aligned}
 \Sigma &= \partial \psi(E, e_p(p)) / \partial E \\
 &= \int_0^1 \sigma(p) dp \\
 &= \Sigma_1 + \Sigma_2 \\
 &= \int_0^{p^*} \sigma_u(p) dp + \int_{p^*}^1 c(p) e dp \\
 &= \Sigma_u \left(1 - \frac{\gamma(\omega, -\ln(1 - p^*))}{\Gamma(\omega)} \right) + (1 - p^*) C_0 E,
 \end{aligned}
 \tag{28}$$

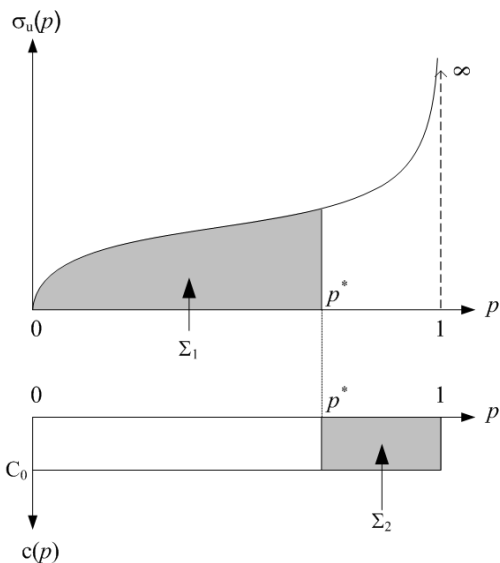


Figure 6. Inverse cdf for the micro thermomechanical one-dimensional plasticity model. (a) microscale strength; (b) microscale elastic modulus.

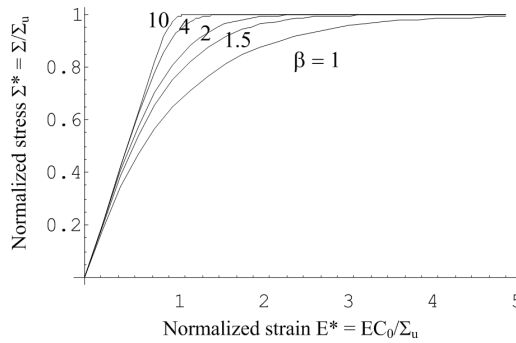


Figure 7. Analytical stress-strain curves for monotonic loading of the one-dimensional randomly distributed plasticity model based on Weibull statistics (in correspondence with Figure 5).

where we use $\omega = 1 + 1/\beta$; Σ_1 and Σ_2 designates the stress contribution from elements on yield or in elastic state; $\gamma(x_1, x_2) = \int_{x_2}^{\infty} \mu^{x_1-1} \exp(-\mu) d\mu$ is the incomplete gamma function; and $p = p^*$ denotes the transition point between those elements. At the transition point, $p = p^*$, both Equations (4) and (25) must be satisfied. Since we seek a solution for proportional monotonic loading conditions $e_p(p \equiv p^*) = 0$ and $C_0E = \sigma_u(p^*)$ such that

$$p^* = 1 - \exp\left[-\left(\frac{\Gamma(\omega)C_0E}{\Sigma_u}\right)^{1/\beta}\right],$$

which upon substitution into Equation (28) gives the analytical solution for monotonic loading conditions of the conceptual one-dimensional model for heterogeneous materials with Weibull’s distribution of strength

$$\frac{\Sigma(E^*)}{\Sigma_u} = 1 - \frac{\gamma(\omega, (E^*\Gamma(\omega))^\beta)}{\Gamma(\omega)} + E^* \exp[-(E^*\Gamma(\omega))^{1/\beta}], \tag{29}$$

where we use $E^* = C_0E/\Sigma_u$. Figure 7 presents the changes in the normalised stress-strain curves resulting from variations in the Weibull’s shape parameter β (corresponding to Figure 5), which decreases with increasing variability in strength. It is clearly shown how a decrease in the strength variability is accompanied with a stronger curvature in the stress-strain curve which seems only logical to expect.

5.2. One-directional cyclic loading of the one-dimensional basic model. The results above were derived for one-directional monotonic loading conditions and analytic expressions were given. However, the model could be reformulated in a numerical form for cyclic loads realisation according to Section 4.4. For this particular model the solution for the n -th nonnegative multiplier takes a rather simple form

$$\tilde{\lambda}_n = \Theta(\sigma_n \dot{E}) |\dot{E}|,$$

where $\Theta(x) = 1$ if $x > 0$, and $\Theta(x) = 0$ if $x \leq 0$. Then according to Equation (17)

$$\dot{\Sigma} = |\dot{E}| \sum_{n=1}^N c(p_n)\omega, \quad \omega = \text{sgn}(\dot{E}) - \Theta(\sigma_n \dot{E}) \text{sgn}(\sigma_n).$$

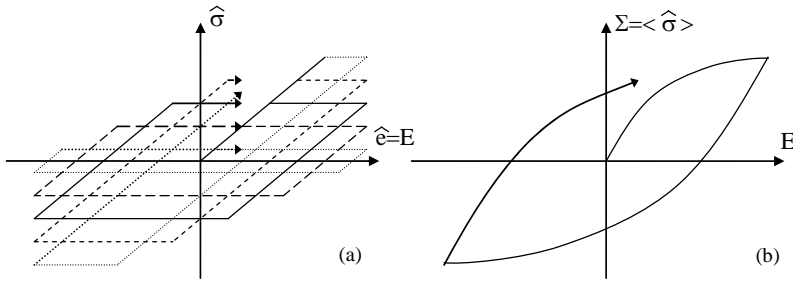


Figure 8. Micro and meso stress-strain curves under cyclic loading conditions of the one-dimensional model.

The last equation (see also a schematic diagram in Figure 8) proves that the model presents the well known Masing hysteretic rules as the microconstituent’s local stiffness multiplier is $\omega = 0, 1, \text{ or } -1$ (for microyield, microelastic loading, or microelastic unloading conditions). The meso stress-strain curve of Figure 8b is defined by integrating the micro stress-strain curves of Figure 8a. Each individual micro stress-strain curve is typical for an elasto-perfectly plastic element, described by a single elastic modulus and a single plastic threshold. Their assembly produces a smooth hysteretic macrocurve without incorporating any kinematic hardening parameter. This model, known as the Masing-Iwan model, could be generalized as we do in the next section.

5.3. Micro thermomechanical von Mises model (with linear elasticity). The previous example model has dealt with the reaction of heterogeneous materials that are subjected to the action of one-directional compression loading. However, the theory can facilitate in defining complete constitutive models that can accommodate any direction of loading. To demonstrate this aspect a conceptual micro thermomechanical von Mises model is derived.

5.3.1. Classical (homogeneous) linear elasto-perfectly plastic von Mises model. The stored elastic energy within linear isotropic elasticity in homogeneous materials is expressed directly by the mesoscopic elastic strains

$$\Psi = \frac{1}{2} (K \cdot \text{tr}(\mathbf{E}_e)^2 + 2G \mathbf{E}_e^d : \mathbf{E}_e^d), \tag{30}$$

where K and G are the bulk and shear moduli; $\text{tr}(\bullet) = \bullet : \mathbf{1}$ is the trace of a second order tensor “ \bullet ” while $\mathbf{1}$ is the second order identity tensor; and we have used $\bullet^d = \bullet - \frac{1}{3} \text{tr}(\bullet) \mathbf{1}$ to denote the distortional (deviatoric) part of the tensor.

The rate of dissipation potential of perfectly plastic von Mises model for homogeneous materials is expressed directly by the mesoscopic plastic strain rates

$$\tilde{\Phi}(\dot{\mathbf{E}}_p) = k \sqrt{2 \dot{\mathbf{E}}_p^d : \dot{\mathbf{E}}_p^d} \geq 0, \tag{31}$$

where k is the simple shear strength. Using the degenerate case Legendre transformation together with $\chi = \Sigma$ resulting from the structure of Equation (30) this potential gives the classical von Mises yield function [Collins and Houlsby 1997]

$$y(\Sigma) = \Sigma^d : \Sigma^d - 2k^2 \leq 0. \tag{32}$$

5.3.2. Von Mises model for randomly distributed heterogeneous materials. It is possible to extend the above homogeneous model within the micro thermomechanics framework. First let us rewrite Equation (30) as a local energy density

$$\psi = \psi_1 = \frac{1}{2}(K_m(p) \cdot \text{tr}(\mathbf{e}_e(p))^2 + 2G_m(p)\mathbf{e}_e^d(p) : \mathbf{e}_e^d(p))$$

thus the global Helmholtz free energy potential is

$$\Psi = \frac{1}{2} \int_0^1 \left(K_m(p) \cdot \text{tr}(\mathbf{E} - \mathbf{e}_p(p))^2 + 2G_m(p)(\mathbf{E}^d - \mathbf{e}_p^d(p)) : (\mathbf{E}^d - \mathbf{e}_p^d(p)) \right) dp, \tag{33}$$

where $K_m(p)$ and $G_m(p)$ are the microscale bulk and shear moduli. It follows that

$$\begin{aligned} \sigma^d(p) &= 2G_m(p)\mathbf{e}_e^d(p), & \text{tr}(\sigma(p)) &= 3K_m(p) \text{tr}(\mathbf{e}_e(p)), \\ \Sigma^d &= \int_0^1 \sigma^d(p) dp = 2 \int_0^1 G_m(p)\mathbf{e}_e^d(p) dp, & \text{tr}(\Sigma) &= 3 \int_0^1 K_m(p) \text{tr}(\mathbf{e}_e(p)) dp. \end{aligned}$$

Let us also rewrite the rate of dissipation potential from Equation (31) in local density form

$$\tilde{\phi}(\dot{\mathbf{e}}_p(p), p) = k_m(p)\sqrt{2\dot{\mathbf{e}}_p^d(p) : \dot{\mathbf{e}}_p^d(p)} \geq 0,$$

where $k_m(p)$ is the simple shear microscale strength. Thus the global potential is

$$\tilde{\Phi}(\dot{\mathbf{e}}_p(p)) = \int_0^1 k_m(p)\sqrt{2\dot{\mathbf{e}}_p^d(p) : \dot{\mathbf{e}}_p^d(p)} dp.$$

Whenever $\dot{\mathbf{e}}_p^d(p) : \dot{\mathbf{e}}_p^d(p) > 0$, the microscale deviatoric stress at point p could also be defined using Equation (17)

$$\sigma^d(p) = 2k_m^2(p)\dot{\mathbf{e}}_p^d(p)/\tilde{\phi}(\dot{\mathbf{e}}_p(p), p),$$

such that $\sigma^d(p) : \sigma^d(p) = 2k_m^2(p)$ and we recover the p -th von Mises yield function in the microscale stress-space

$$y(\sigma(p), p) = \sigma^d(p) : \sigma^d(p) - 2k_m^2(p) \leq 0$$

which in the mesoscale strain-space is written by

$$y(\mathbf{E}, \mathbf{e}_p(p), p) = 2G^2(p)\mathbf{e}_e^d(p) : \mathbf{e}_e^d(p) - k_m^2(p) = 2G^2(p)(\mathbf{E}^d - \mathbf{e}_p^d(p)) : (\mathbf{E}^d - \mathbf{e}_p^d(p)) - k_m^2(p) \leq 0.$$

Instantaneous elasticity. From (23), (24) and (33) the instantaneous macro shear and bulk moduli is

$$G = \int_0^1 G_m(p) dp = \langle \hat{G} \rangle, \quad K = \int_0^1 K_m(p) dp = \langle \hat{K} \rangle.$$

Terminal mesoscale yielding. Let us define terminal mesoscale yielding when all the subelements constituents yield, that is, when $\sigma^d(p) : \sigma^d(p) = 2k_m^2(p)$ for any p . The solution for the microscale deviatoric stress is in the form

$$\sigma^d(p) = \sqrt{2}k_m(p)\mathbf{n}', \quad \text{where } \mathbf{n}' : \mathbf{n}' = 1, \text{ and } \mathbf{n}' : \mathbf{1} = 0. \tag{34}$$

If $\sigma^d(p) : \sigma^d(p) = 2k_m^2(p)$ is satisfied for any p , its integral form is satisfied as well, thus

$$\int_0^1 \sqrt{\sigma^d(p) : \sigma^d(p)} dp = \langle \sqrt{\hat{\sigma}^d : \hat{\sigma}^d} \rangle = \sqrt{2}\bar{k},$$

where we designate the constant $\bar{k} = \int_0^1 k_m(p) dp$. A question arises as to whether \bar{k} agrees with the constant k of the conventional (homogeneous) von Mises model. From Equation (32) upon yielding the conventional von Mises model predicts

$$\sqrt{\Sigma^d : \Sigma^d} = \sqrt{\langle \hat{\sigma}^d \rangle : \langle \hat{\sigma}^d \rangle} = \sqrt{2}k,$$

which with Equation (34) proves that $\bar{k} = k$, thus the overall mesoscale simple shear strength is given by the average over the microscale simple shear strengths in the SVE

$$k = \int_0^1 k_m(p) dp = \langle \hat{k}_m \rangle.$$

6. Evaluation of the probabilistic approach

In the previous sections the different properties in the modelling approach were physically interpreted. The suitability of this interpretation is dependent on the validity of the probabilistic concepts adopted in Section 2. For that purpose this section presents a short numerical study. This study includes several finite difference (FD) experiments using the commercial code FLAC of Itasca [FLAC 2000], which are compared with the analytical solution of the same problem based on the micro thermomechanics framework. The advantages of the use of FLAC for such analyses was recently noticed by Ostoja-Starzewski [2005], who have performed similar calculations for rigid-perfectly-plastic two-phase randomly distributed medium. This paper will concern itself with materials with finite rigidity that are presented for continuous phased Weibull media.

The FD models in our calculations involve a 50×50 element mesh that represents 2500 von Mises subelements in a single RVE. The large number of elements used for the analyses was chosen such that the simulation will satisfy, as close as possible, the criterion of $\delta = L/l = 50 \rightarrow \infty$ in order to be able to consider results from a point statistics view point. As a result we can practically view the RVE as a SVE with the weaker form of nondimensional length scales. According to Ostoja-Starzewski [2005], when δ tends to infinity, results for constant applied displacement or constant applied traction boundary conditions tend to merge to a unique solution for a given deterministic spatial arrangement of a randomly distributed material. Thus the following calculations will be based only on applying constant displacement boundary conditions. The bulk modulus received a significantly large value insuring that the calculation will simulate as close as possible the behaviour of incompressible material. This condition insures that a plane strain FD model with constant vertical and horizontal displacements but with opposite signs acting on the horizontal and vertical boundaries will not produce a stress reaction perpendicular to the plane. This point was validated during the calculation by averaging the in-plane stresses in all the subelements and validating that the result is negligible compared to the other stress components. The mesoscale vertical and horizontal stresses acting on the horizontal and vertical boundaries were calculated by summing the unbalanced forces along the corresponding boundaries and dividing them by their lengths. The mesoscale vertical strain was calculated simply by dividing the vertical relative

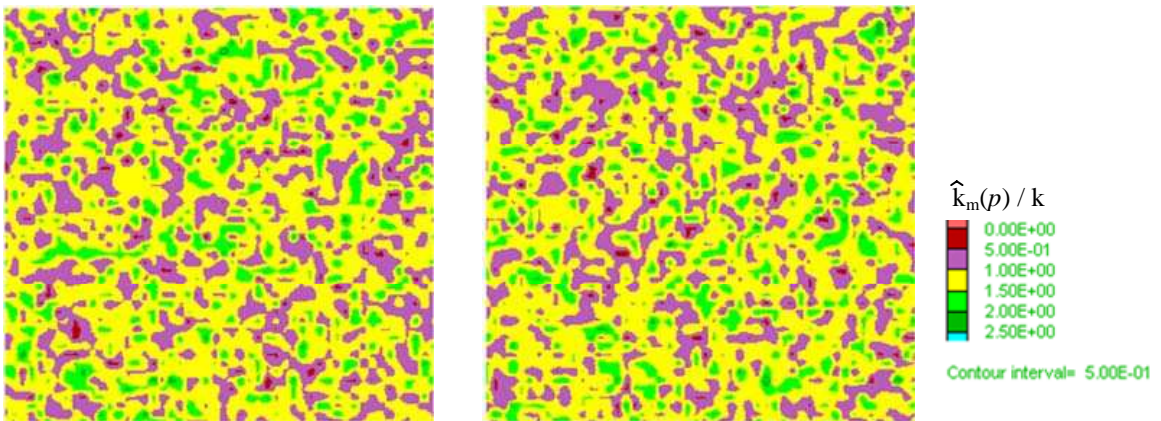


Figure 9. Contours of the normalized von Mises strength distribution ($\hat{k}_m(p)/k$) within two randomly based 50*50 elements FLAC experiments generated by the Weibull inverse cdf.

displacement between the horizontal boundaries by their distance. The opposite operation gave the mesoscale horizontal strain.

6.1. Monotonic loads on Weibullian random elasto-plastic von Mises media. Weibull's statistics is most appropriate in describing the spatial variations in the compression strength of materials (for example as demonstrated by McDowell and Bolton [1998] for sands) and it is not so clear whether such a distribution may also be appropriate in describing variations in the shear strength. However, our main purpose is to assess the theoretical assumptions and this could be more easily done by randomly varying the shear strength coefficients between the (von Mises) subelements. To this end using a modification to Equation (26)) Weibull's inverse cdf is used for generating spatial variations in the simple shear strength $k_m(p) = k[-\ln(1-p)]^{1/\beta}/\Gamma(1+1/\beta)$, while the shear and bulk stiffness moduli $G_m(p) = G$ and $K_m(p) = K \gg G$ were homogeneous. In the analyses the range of $\beta = 1.5, 3, 10$ will be used to cover ideal materials ranging from strongly ($\beta = 1.5$, typical low value for silica sand [Nakata et al. 1999]) to weakly heterogeneous materials ($\beta = 10$, typical for ceramics [Espinosa et al. 2003]). Each ideal material will be analyzed based on two deterministic fields thus giving a total of 6 analyses. This means that the two FD calculations for the same β material are essentially different in their geometrical configuration. This is illustrated in Figure 9, describing the contours of two different deterministic fields of the normalized microscale von-Mises strength within the first and second FLAC calculations for the same $\beta = 3$ randomly distributed material.

Our aim is to show that the results from the finite difference calculations do not change practically if we use the same random distribution to obtain a different deterministic arrangement. This is carried out to validate the proposition of the MPR. The results from the 6 different FLAC calculations are presented in Figure 10. It is clearly shown that the responses are repetitive. The minor discrepancies between the lines can be largely attributed to the fact that only 2500 subelements were used, while point statistic requires essentially infinite number.

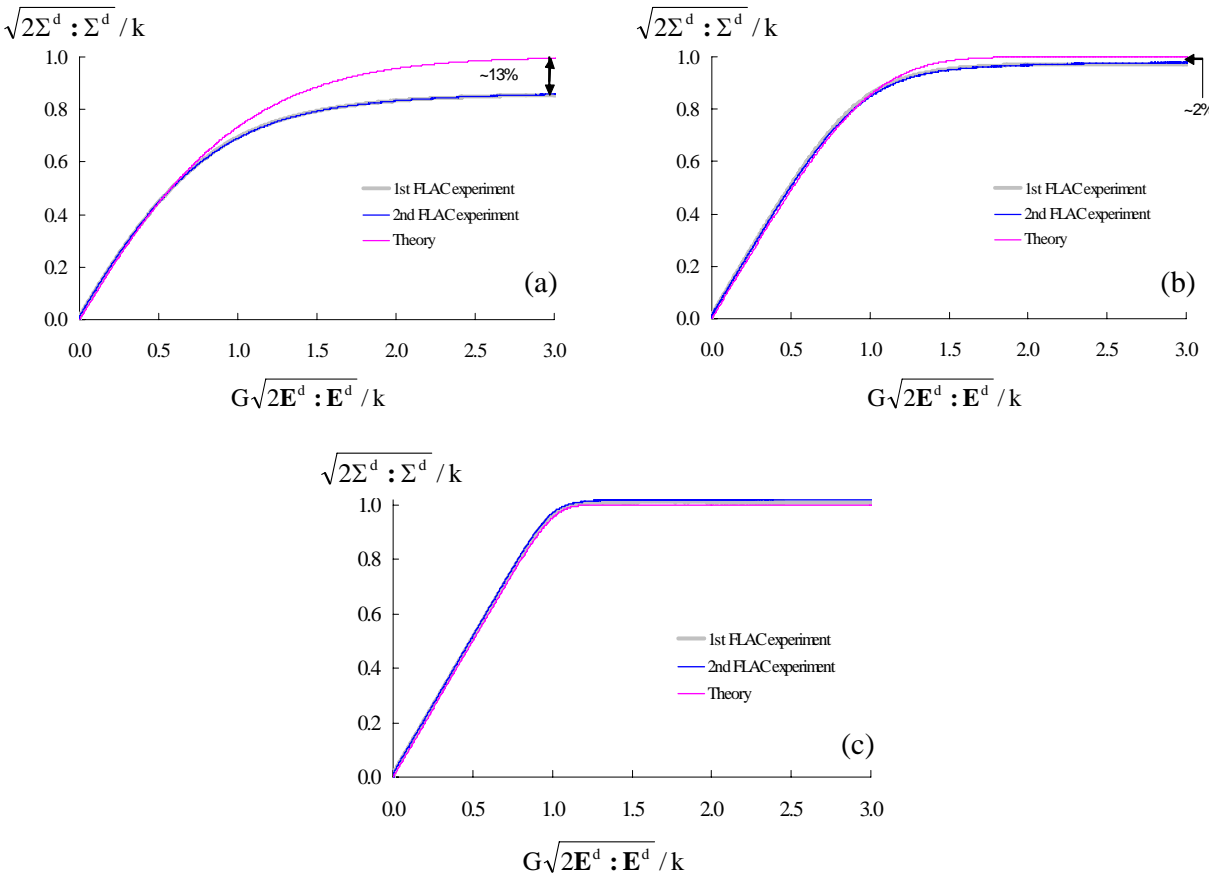


Figure 10. Comparison between 2 different deterministic FLAC experiments and the theoretical expression for (a) $\beta = 1.5$, (b) $\beta = 3$, and (c) $\beta = 10$ materials.

Next, we will evaluate the ability of the theoretical framework to predict the same results. Applying the back-bone curve of the one-dimensional model given Equation (29) to the general Von Mises model for randomly distributed heterogeneous materials suggests that in the current loading condition

$$J^*_1 = 1 - \frac{\Gamma(\omega, (J^*_2 \Gamma(\omega))^\beta)}{\Gamma(\omega)} + J^*_2 \exp[-(J^*_2 \Gamma(\omega))^{1/\beta}],$$

where

$$J^*_2 = \frac{G\sqrt{2\mathbf{E}' : \mathbf{E}'}}{k} \quad \text{and} \quad J^*_1 = \frac{\sqrt{\frac{1}{2}\mathbf{\Sigma}' : \mathbf{\Sigma}'}}{k}.$$

The predictions from the above equation are compared with the 2500 elements FD calculations; these are given in the Figure 10. The agreement is quantitatively very good and qualitatively excellent. Nevertheless it should be mentioned that the analytical solution gives a stiffer response. The difference is reduced as the degree of heterogeneity is reduced from approximately 13% difference in the highly heterogeneous case of $\beta = 1.5$ down as β increases. When $\beta = 10$ the numerical prediction is even

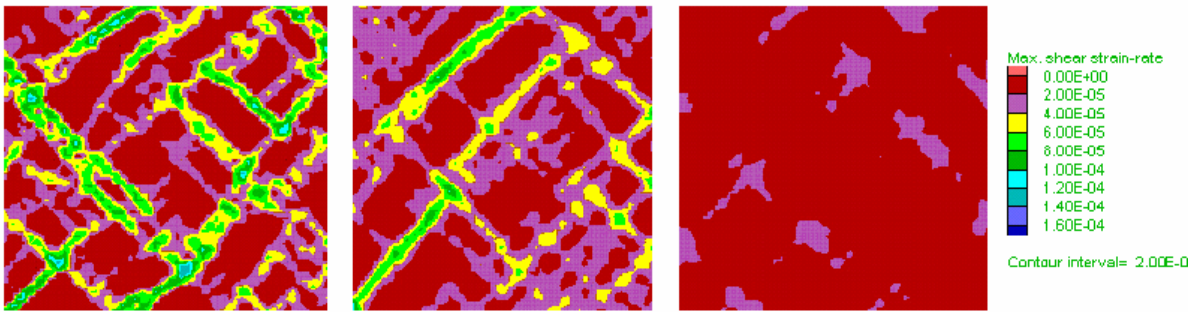


Figure 11. Internal patterning of deformations (maximum shear strain-rate) for a single deterministic calculation using $\beta = 1.5, 3,$ and 10 materials.

showing a fractionally stiffer response, but this is attributed to dynamical wave propagation numerical drift in FLAC due to a shock in the early beginning of the calculation. This shock was eliminated as much as possible by ramping the load slowly.

In order to reduce the deviation of the theory from the true solution future improvements should include better estimates than the uniform strain assumption. This issue is highlighted when examining the internal patterning of deformations by plotting the maximum shear strain rate contours. As is shown in Figure 11 scattered shear bands appears in a random fashion. As expected those bands are deviated 45° from the horizon with some noise due to the randomness of the field. Theoretically, if the subelement size l was reduced to infinitesimal normalized size compared with L , those bands should tend to be infinitesimally thin slip lines as suggested by Ostoja-Starzewski and Ilies [1996]. Based on Figure 11 it can also be observed that as the degree of heterogeneity is reduced, the average distance between the slip lines is increasing. One possibility for further improvements would be to introduce an additional (normalized) length scale denoting the average distance between the slip lines. Alternatively, possibly a better option could be to introduce additional distribution function denoting the probability of a particular subelement to be within a slip line.

6.2. Cyclic loads on Weibullian random elasto-plastic von Mises media. Next the same FD model is examined under cyclic loading conditions (for the $\beta = 3$ case only). After applying deviatoric load in a similar manner to the previous section, the direction of the boundary displacements is reversed followed by another (re)loading phase. This cyclic loading test requires a very careful numerical procedure in which a sinusoidal type of ramping is applied minimizing the numerical dynamics waves as much as possible. The response of the detailed FD model is compared against the prediction of the simple micro thermomechanical von Mises constitutive model in Figure 12. The response of the simple model could be derived either by utilising the numerical discretisation method or simply by applying Masing rules on the approximating analytical formula (1). It is shown that the simple constitutive model agrees rather well with the detailed numerical FD model.

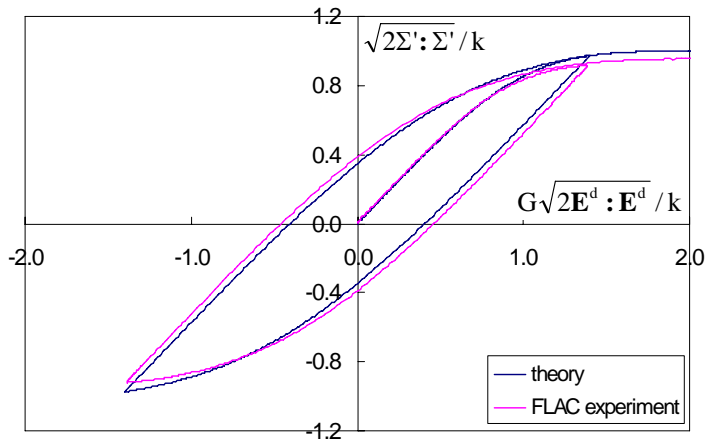


Figure 12. Comparison between the FLAC experiment and the performance of the constitutive model under unidirectional cyclic load for $\beta = 3$.

7. Summary

A theory for modelling heterogeneous randomly distributed elastic-plastic materials was presented. A conventional thermomechanical elasto-plastic constitutive modelling framework is proposed but one that allows an effective physical interpretation of the micromechanical internal variables and inherent parameters in a RVE. The main points behind this work are as follow

1. The paper demonstrates a micro thermomechanical constitutive modelling methodology that allows deriving estimates for the response of random elasto-plastic material under monotonic, cyclic and multidirectional loads. This particular property of the framework enables to capture memory features that are intrinsic within plastic material.
2. The method of probabilistic rearrangement (MPR) is suggested and verified against the finite Difference program of FLAC. By applying the MPR conventional constitutive modelling frameworks could be linked directly to the statistical distribution of the elasto-plastic material properties within the RVE or a SVE. The MPR enables to estimate effective properties within the SVE such that mesoscopic as well as microscopic field variables could be evaluated using localisation-homogenisation analytical procedure. An important point is that the MPR allows accounting for the gradual yielding that occurs within the SVE; a fact that could not be accounted for if the set of infinite plastic internal variables are replaced by a single average plastic internal variable.
3. The MPR facilitated in recovering analytical approximating formula to monotonic loading conditions of the full probabilistic boundary value problem. Under one-directional cyclic loading conditions, the approximating analytical formula could be extended using the famous Masing rules to provide the estimate of the micro thermomechanical constitutive model to the full probabilistic boundary value problem. For the more complicated scenarios of general multidirectional cyclic loading conditions a simple numerical procedure is suggested.

4. The results for the cyclic loading case show how hysteresis behavior of random materials could be realized directly by describing the physical heterogeneities in the material properties without the need to incorporate any kinematic hardening parameters.

8. Acknowledgments

The authors would like to acknowledge Prof. Arcady Dyskin from The University of Western Australia And Prof. Andrew Drescher from University of Minnesota for their valuable comments. Furthermore, support for the first author from the Australian Research Council through the ARC Discovery grant scheme (DP0558406) is gratefully acknowledged.

References

- [Adams et al. 1989] B. L. Adams, G. R. Canova, and A. Molinari, "A statistical formulation of viscoplastic behaviour in heterogeneous polycrystals", *Textures Microstruct.* **11** (1989), 57–71.
- [Chaboche 2003] J. L. Chaboche, "Thermodynamics of local state: overall aspects and micromechanics based constitutive relations", pp. 113–129 in *Technische Mechanik*, Manuskripteingang, 11. Juni 2003 2003. Band 23, Heft 2–4.
- [Chang and Ma 1991] C. S. Chang and L. Ma, "A micromechanically-based micropolar theory for deformation of granular solids", *Int. J. Solids Struct.* **28**:1 (1991), 67–86.
- [Collins 2005a] I. F. Collins, "Elastic/plastic models for soils and sands", *Int. J. Mech. Sci.* **47** (2005a), 493–508.
- [Collins 2005b] I. F. Collins, "The concept of "stored plastic work" or "frozen elastic energy" in soil mechanics", *Geotechnique* **55**:5 (2005b), 373–382.
- [Collins and Hilder 2002] I. F. Collins and P. A. Hilder, "A theoretical framework for constructing elastic/plastic constitutive models of triaxial tests", *Geotechnique* **52**:7 (2002), 507–518.
- [Collins and Houlsby 1997] I. F. Collins and G. T. Houlsby, "Application of thermomechanical principles to the modeling of geomaterials", *Proc. R. Soc. Lon. Ser-A* **453** (1997), 1975–2001.
- [Collins and Kelly 2002] I. F. Collins and P. A. Kelly, "A thermomechanical analysis of a family of soil models", *Geotechnique* **52**:7 (2002), 507–518.
- [Collins and Muhunthan 2003] I. F. Collins and B. Muhunthan, "On the relationship between stress-dilatancy, anisotropy, and plastic dissipation for granular materials", *Geotechnique* **53**:7 (2003), 611–618.
- [Cundall and Strack 1979] P. A. Cundall and O. D. L. Strack, "A discrete model for granular assemblies", *Geotechnique* **29**:7 (1979), 47–65.
- [Doghri 2000] I. Doghri, *Mechanics of deformable solids. Linear, nonlinear, analytical and computational aspects*, Springer, Berlin, 2000.
- [Drescher and de Josselin de Jong 1972] A. Drescher and G. de Josselin de Jong, "Photoelastic verification of a mechanical model for the flow of a granular material", *J. Mech. Phys. Solids* **20** (1972), 337–351.
- [Einav 2002] I. Einav, *Applications of thermodynamical approaches to mechanics of soils*, PhD. Thesis, Technion- Israel Institute of Technology, Haifa, 2002.
- [Einav 2005] I. Einav, "A second look at strain space plasticity and latest applications", pp. 225–231 in *18th Australasian conference on the mechanics of structures and materials (ACMSM)*, vol. 1, Perth, 1–3 December 2005.
- [Einav and Puzrin 2004] I. Einav and A. M. Puzrin, "Continuous hyperplastic critical state (CHCS) model: derivation", *Int. J. Solids Struct.* **41**:1 (2004), 199–226.
- [Espinosa and Zavattieri 2003] H. D. Espinosa and P. D. Zavattieri, "A grain level model for the study of failure initiation and evolution in polycrystalline brittle materials. Part I: theory and numerical implementation", *Mech. Mater.* **35** (2003), 333–364.
- [Espinosa et al. 2003] H. D. Espinosa, B. Peng, B. C. Prorok, N. Moldovan, O. Auciello, J. A. Carlisle, D. M. Gruen, and D. C. Mancini, "Fracture strength of ultrananocrystalline diamond thin films- identification of Weibull parameters", *J. Appl. Phys.* **94**:9 (2003), 6076–6084.

- [FLAC 2000] *FLAC (Fast Lagrangian Analysis of Continua) User's Manual*, Itasca Consulting Group, Inc., Minneapolis Minnesota: Itasca, 2000. Ver. 4.0.
- [Frantziskonis 1998] G. Frantziskonis, "Stochastic modelling of heterogeneous materials- A process for the analysis and evaluation of alternative formulations", *Mech. Mater.* **27**:3 (1998), 165–175.
- [Garmestani et al. 1988] H. Garmestani, S. Lin, and B. L. Adams, "Statistical continuum theory for inelastic behaviour of a two-phase medium", *Int. J. Plasticity* **14**:8 (1988), 719–731.
- [Gurtin 2000] M. E. Gurtin, "On the plasticity of single crystals: free energy, microforces, plastic-strain gradients", *J. Mech. Phys. Solids* **48** (2000), 989–1036.
- [Hill 1963] R. Hill, "Elastic properties of reinforced solids: some theoretical principles", *J. Mech. Phys. Solids* **11** (1963), 357–372.
- [Houlsby and Puzrin 2000] G. T. Houlsby and A. M. Puzrin, "A thermomechanical framework for constitutive models for rate-independent dissipative materials", *Int. J. Plasticity* **16**:9 (2000), 1017–1047.
- [Houlsby and Sharma 1999] G. T. Houlsby and R. S. Sharma, "A conceptual model for the yielding and consolidation of clays", *Geotechnique* **49**:4 (1999), 491–502.
- [Maugin 1992] G. A. Maugin, *The thermomechanics of plasticity and fracture*, Cambridge University Press, 1992.
- [McDowell and Bolton 1998] G. R. McDowell and M. D. Bolton, "On the micro mechanics of crushable aggregates", *Geotechnique* **48**:5 (1998), 667–679.
- [Nakata et al. 1999] Y. Nakata, A. F. L. Hyde, M. Hyodo, and H. Murata, "A probabilistic approach to sand particle crushing in the triaxial test", *Geotechnique* **49**:5 (1999), 567–583.
- [Ostoja-Starzewski 2002] M. Ostoja-Starzewski, "Microstructural randomness versus representative volume element in thermomechanics", *J. Appl. Mech. (Trans. ASME)* **69** (2002), 25–35.
- [Ostoja-Starzewski 2005] M. Ostoja-Starzewski, "Scale effects in plasticity of random media: status and challenges", *Int. J. Plasticity* **21** (2005), 1119–1160.
- [Ostoja-Starzewski and Ilies 1996] M. Ostoja-Starzewski and H. Ilies, "The Cauchy and characteristic boundary value problems of random rigid-perfectly plastic media", *Int. J. Solids Struct.* **33**:8 (1996), 1119–1136.
- [Pasternak and Mühlhaus 2005] E. Pasternak and H.-B. Mühlhaus, "Generalised homogenisation procedures for granular materials", *J. Eng. Math.* **52**:1 (2005), 199–229(31).
- [Ponte Castañeda 1996] P. Ponte Castañeda, "Exact second-order estimates for the effective mechanical properties of nonlinear composite materials", *J. Mech. Phys. Solids* **44**:6 (1996), 827–862.
- [Puzrin and Houlsby 2001] A. M. Puzrin and G. T. Houlsby, "A thermomechanical framework for rate-independent dissipative materials with internal functions", *Int. J. Plasticity* **17** (2001), 1147–1165.
- [Puzrin et al. 2001] A. M. Puzrin, G. T. Houlsby, and J. B. Burland, "Thermomechanical formulation of a small strain model for overconsolidated clays", *Proc. R. Soc. Lon. Ser-A* **457**:2006 (February 2001), 425–440. ISSN 1364-5021.
- [Rice 1971] J. R. Rice, "Inelastic constitutive relations for solids: an internal variable theory and its application to metal plasticity", *J. Mech. Phys. Solids* **19** (1971), 433–455.
- [Satake 1978] M. Satake, "New formulation of graph-theoretical approach in the mechanics of granular materials", *Mechanics of Materials* **16(1-2)** (1978), 65–72.
- [Suquet 1987] P. M. Suquet, "Elements of homogenization for inelastic solid mechanics", pp. 194–271 in *Proc. Homogenization Techniques for Composite Media, Udine, Italy 1985*, 272, Part IV, Springer-Verlag, 1987. Lecture Notes in Physics.
- [Tordesillas et al. 2004] A. Tordesillas, S. D. C. Walsh, and B. Gardiner, "Bridging the length scales: micromechanics of granular media", *BIT Numerical Mathematics* **44** (2004), 539–556.
- [Ulm and Coussy 2003] F.-J. Ulm and O. Coussy, *Mechanics and durability of solids*, vol. 1, Prentice Hall, New Jersey, 2003.
- [Vardoulakis 1983] I. Vardoulakis, "Rigid granular plasticity model and bifurcation in the triaxial test", *Acta Mech.* **49** (1983), 57–79.
- [Vardoulakis and Sulem 1995] I. Vardoulakis and J. Sulem, *Bifurcation analysis in geomechanics*, Blackie Academic and Professional, 1995.

- [Walsh and Tordesillas 2004] S. D. C. Walsh and A. Tordesillas, "A thermomechanical approach to the development of micropolar constitutive models for granular media", *Acta Mech.* **167**:3-4 (2004), 145–169.
- [Walton 1987] K. Walton, "The effective elastic moduli of a random packing of spheres", *J. Mech. Phys. Solids* **35**:2 (1987), 213–226.
- [Weibull 1951] W. Weibull, "A statistical distribution function of wide applicability", *J. Appl. Mech. (Trans. ASME)* **18** (1951), 293–297.
- [Ziegler 1977] H. Ziegler, *An introduction to thermomechanics*, 2nd edition: 1983 ed., North Holland, Amsterdam, 1977.

Received 16 Sep 2007. Accepted 10 Dec 2007.

ITAI EINAV: I.Einav@civil.usyd.edu.au

School of Civil Engineering, The University of Sydney, Sydney, NSW 2006, Australia

IAN F. COLLINS: i.collins@auckland.ac.nz

Department of Engineering Science, The University of Auckland, Auckland 1142, New Zealand