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A multiscale approach for the micropolar continuum model

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Abstract: A method to derive governing equations and elastic-plastic constitutive relations for the micropolar continuum model is proposed. Averaging procedures are operated over a surrounding sub-domain for each material point to bridge a discrete microstructure to a macro continuum model. Material parameters are determined by these procedures. The size of the sub-domain represents the material intrinsic length scale, and it is passed into the macroscopic governing equation so that the numerical solution can be regularized for analyses of failure phenomena. An application to a simple granular material model is presented.

keyword: micropolar continuum, material parameter, failure analysis, microstructure

1 Introduction

In failure phenomena of rate-independent strain-softening materials, deformation often localizes in a very small portion of the entire domain. The existing computational methods within the framework of conventional continuum mechanics such as the finite element method (FEM) are not always applicable to these problems, because one may encounter significant mesh dependence. For example, in a one-dimensional problem, the plastic strain localizes in one element after the failure no matter how fine the finite element mesh is. To avoid this spuriously mesh-dependent result, it is known that one of the regularization methods is required (Belytschko, Liu, and Moran, 2000). In addition, to capture the localized strain distribution, very fine discretization is required. Finite elements should be much smaller than the size of the localized region.

In the late 1980's, regularization methods were developed intensively and are reviewed in Belytschko, Liu, and Moran (2000) such as the non-local model (Bažant and Belytschko, 1985; Bažant, Belytschko, and Chang, 1984), the gradient model (Lasry and Belytschko, 1988), the couple stress model (Mühlhaus and Vardoulakis, 1987), and the rate-dependent model (Needleman, 1988). These regularization methods embed a length scale in the governing equations directly or indirectly. Among these regularization methods, the couple stress approach is focused on in this paper. Germain (1973) formulated the weak form governing equations for the micromorphic continuum model of Eringen and Suhubi (1964). Mühlhaus and Vardoulakis (1987) derived the shear stress invariant and the plastic shear strain invariant including the couple stress and the micro curvature by averaging the slip among the microstructure of a granular material. De Borst (1993) generalized the J_2-flow theory with the couple stress and the micro curvature. This theory has been applied to static and dynamic problems (de Borst, 1993; de Borst, Sluys, Mühlhaus, and Pamin, 1993) . Recently, thermo-visco-elastic constitutive equations for the micropolar continuum model were derived by Chen, Lee, and Eskandarian (2004), and an overview of the polar theory is shown there. However, how to determine the material parameters for the constitutive relations and the size of the length scale has been an open question. In order to bridge the discrete microstructure to the continuum, these should reflect the material microstructure which conventional continuum mechanics cannot represent. Since the late 1990's, it is studied by many researchers to incorporate higher order gradient of displacement into the continuum mechanics. For example, Kouznetsova, Geers, and Brekelmans (2002) developed a multi-scale constitutive modeling technique using the numerical homogenization method, and Gao, Huang, Nix, and Hutchinson (1999) enhanced the plasticity theory with strain gradients.

To decrease the computational cost, graded mesh is a common method for the analyses of localized phenomena. However, in dynamic analyses, one may encounter

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spurious wave reflection at the transition point of mesh density. Also, the time step is restricted by the smallest elements. To enhance the computational efficiency without sacrificing the accuracy, a class of computational method has been developed. Liu, Uras, and Chen (1997) developed the so-called bridging scale method that enriches FEM with a meshfree method. This method has been extended to couple molecular dynamics computations and FEM (Wagner and Liu, 2003; Wagner, Karpov, and Liu, 2004; Karpov, Wagner, and Liu, 2005; Liu, Karpov, Zhang, and Park, 2004; Park and Liu, 2004; Park, Karpov, Liu, and Klein, 2005) . Also, coupling of two FEM computations of different resolution, fine-scale FEM and coarse-scale FEM, has been developed for the micropolar continuum model using this method (Kadowaki and Liu, 2004). This method connects two numerical analyses running simultaneously by an imposed dynamic interface condition. This condition is derived assuming the periodicity of the fine-scale FEM mesh based on the Fourier analysis of repetitive structures (Karpov, Stephen, and Dorofeev, 2002; Karpov, Stephen, and Liu, 2003). By this method, spurious wave reflection can be suppressed and one can use different time steps in the fine-scale FEM and the coarse-scale FEM.

In this study, an approach taken to determine material parameters for the micropolar continuum is proposed and example problems are computed by the bridging scale method with two FEM meshes (Kadowaki and Liu, 2004). The main focus is on the approach to determine the material parameters. It is based on some of the existing works mentioned above. The major distinction is that both the governing equations and the constitutive relations of the proposed model are derived by averaging over a surrounding sub-domain which is motivated by the approach of Gao, Huang, Nix, and Hutchinson (1999) and Mühlhaus and Vardoulakis (1987). Both the virtual internal power and invariants for plastic deformation at a macroscopic material point are expressed by the average over the surrounding sub-domain, which represents the extent of the influence from neighboring material points. Thus, this sub-domain is called *the domain of influence* (DOI). The main advantage of this approach is that the formulation embeds the size of the DOI into the governing equations, yields the relationship between the elastic parameters, and determines the parameters for the plastic constitutive relations.

In section 2, the micropolar continuum model and the generalized J_2-flow theory are reviewed. In section 3, the proposed multiscale approach is explained. In section 4, an elastic-plastic constitutive relation is presented for a simple granular material model. In section 5, numerical examples are presented. In section 6, concluding remarks are made.

2 Review of the micropolar continuum model and the generalized J_2-flow theory

2.1 Governing equations

Let u_i and $\dot{u}_i$ denote the displacement field and the velocity field, respectively. A superposed dot denotes the material time derivative. The micropolar continuum model includes a skew-symmetric second order tensor $\dot{\omega}_{ij}$ which is called micro-spin. Both $\dot{u}_i$ and $\dot{\omega}_{ij}$ are functions of the material coordinate $\mathbf{X}$ and time t. Let Ω and Γ denote the current domain and its boundary, respectively. The current position of a material point $\mathbf{X}$ is denoted by $\mathbf{x}$. Consider a virtual velocity field $\delta\dot{u}_i$ and a virtual micro-spin field $\delta\dot{\omega}_{ij}$. Following Germain (1973), the virtual kinetic power of the micropolar continuum model δP^{kin} can be written as follows:

$$\delta P^{\text{kin}} = \int \rho \ddot{u}_i \delta\dot{u}_i + \rho I \ddot{\omega}_{ij} \delta\dot{\omega}_{ij} d\Omega \tag{1}$$

where ρ and ρI denote the density and the inertia of the micro-rotation per unit volume. The derivation of the virtual kinetic power is shown in the appendix.

Let L_{ij} denote the macro-velocity gradient defined as

$$L_{ij} = \frac{\partial \dot{u}_i}{\partial x_j} \tag{2}$$

where x_i denotes the spatial coordinate. Let the symmetric part and the skew-symmetric part of L_{ij} be denoted by D_{ij} and W_{ij}, respectively. The virtual internal power δP^{int} is assumed to be linearly dependent on the macro-velocity-gradient, the micro-spin, and the gradient of the micro-spin as

$$\delta P^{\text{int}} = \int \sigma^{\text{S}}_{ji} \delta D_{ij} + \sigma^{\text{A}}_{ji} (\delta\dot{\omega}_{ij} - \delta W_{ij}) + \tau_{kji} \delta\dot{\omega}_{ij,k} d\Omega \tag{3}$$

where a comma in a subscript denotes the spatial derivative. The stress measures σ^{S}_{ji}, σ^{A}_{ji}, and τ_{kji} are called the macro-stress, the micro-stress, and the couple stress respectively. Note that because of the symmetric or skew-symmetric properties of these stress measures,

$$\begin{aligned} \sigma^{\mathrm{S}}_{ji} &= \sigma^{\mathrm{S}}_{ij} \\ \sigma^{\mathrm{A}}_{ji} &= -\sigma^{\mathrm{A}}_{ij} \\ \tau_{kji} &= -\tau_{kij} \end{aligned} \tag{4}$$

It is also assumed that the virtual external power $\delta P^{\,\mathrm{ext}}$ can be written as

$$\delta P^{\,\mathrm{ext}} = \int b_i \delta \dot{u}_i + \Phi_{ji} \delta \dot{\omega}_{ij} \mathrm{d}\Omega + \int t_i \delta \dot{u}_i + T_{ji} \delta \dot{\omega}_{ij} \mathrm{d}\Gamma \tag{5}$$

Body force and body couple are denoted by b_i and Φ_{ji}, respectively. Surface traction and surface moment are denoted by t_i and T_{ji}, respectively. The first terms in each integration on the right hand sides of Eq. (1), Eq. (3), and Eq. (5) are the same as those of conventional continua. Additional terms are introduced by the micropolar continuum model.

Define boundaries Γ^u, Γ^t, Γ^ω, and Γ^T as the boundary of prescribed velocity, traction, micro-spin, and surface moment, respectively, such that

$$\begin{aligned} \Gamma^u \cup \Gamma^t = \Gamma \quad &, \quad \Gamma^u \cap \Gamma^t = 0 \\ \Gamma^\omega \cup \Gamma^T = \Gamma \quad &, \quad \Gamma^\omega \cap \Gamma^T = 0 \end{aligned} \tag{6}$$

The essential boundary conditions can be written as

$$\begin{aligned} \dot{u}_i = \dot{u}^0_i \quad & \text{on } \Gamma^u \\ \dot{\omega}_{ij} = \dot{\omega}^0_{ij} \quad & \text{on } \Gamma^\omega \end{aligned} \tag{7}$$

where $\dot{u}^0_i$ and $\dot{\omega}^0_{ij}$ are the prescribed velocity and micro-spin on the boundaries, respectively. Assume that the condition for the trial functions $\dot{u}_i$, and $\dot{\omega}_{ij}$ are as follows:

$$\begin{aligned} & \dot{u}_i(\mathbf{X},t) \in U \\ & U = \left\{ \dot{u}_i(\mathbf{X},t) \middle| \dot{u}_i \in C^0(\mathbf{X}), \dot{u}_i(\mathbf{X},t) = \dot{u}^0_i(t) \text{ on } \Gamma^u \right\} \\ & \dot{\omega}_{ij}(\mathbf{X},t) \in V \\ & V = \left\{ \dot{\omega}_{ij}(\mathbf{X},t) \middle| \dot{\omega}_{ij} \in C^0(\mathbf{X}), \dot{\omega}_{ij}(\mathbf{X},t) = \dot{\omega}^0_{ij}(t) \text{ on } \Gamma^\omega \right\} \end{aligned} \tag{8}$$

Similarly, assume the condition for the test functions $\delta\dot{u}_i$ and $\delta\dot{\omega}_{ij}$ as follows:

$$\begin{aligned} & \delta\dot{u}_i(\mathbf{X}) \in U_0 \\ & U_0 = \left\{ \delta\dot{u}_i(\mathbf{X}) \middle| \dot{u}_i \in C^0(\mathbf{X}), \delta\dot{u}_i = 0 \text{ on } \Gamma^u \right\} \\ & \delta\dot{\omega}_{ij}(\mathbf{X},t) \in V_0 \\ & V_0 = \left\{ \dot{\omega}_{ij}(\mathbf{X},t) \middle| \dot{\omega}_{ij} \in C^0(\mathbf{X}), \delta\dot{\omega}_{ij} = 0 \text{ on } \Gamma^\omega \right\} \end{aligned} \tag{9}$$

The principle of virtual power states that

$$\begin{aligned} 0 = \delta P^{\,\mathrm{kin}}(t) + \delta P^{\,\mathrm{int}}(t) - \delta P^{\,\mathrm{ext}}(t) \\ \forall \delta\dot{u}_i(\mathbf{X}), \delta\dot{\omega}_{ij}(\mathbf{X},t) \end{aligned} \tag{10}$$

Integrating Eq. (10) by parts and applying the divergence theorem, one can obtain the strong form for the governing equations and the natural boundary conditions as follows:

$$\begin{aligned} \rho \ddot{u}_i - (\sigma^{\mathrm{S}}_{ji} - \sigma^{\mathrm{A}}_{ji})_{,j} = b_i \quad & \text{in } \Omega \\ \rho I \ddot{\omega}_{ij} + (\sigma^{\mathrm{A}}_{ji} - \tau_{kji,k}) = \Phi_{ji} \quad & \text{in } \Omega \end{aligned} \tag{11}$$

$$\begin{aligned} (\sigma^{\mathrm{S}}_{ji} - \sigma^{\mathrm{A}}_{ji}) n_j = t_i \quad & \text{on } \Gamma^t \\ \tau_{kji} n_k = T_{ji} \quad & \text{on } \Gamma^T \end{aligned} \tag{12}$$

where n_i is the unit normal vector on the boundaries. The arguments about the material coordinate $\mathbf{X}$ and time t are omitted for simplicity.

2.2 Constitutive relation with the generalized J_2-flow theory

Similar to the generalized J_2-flow theory of de Borst (1993), the elastic constitutive law is assumed to have the following forms:

$$\begin{aligned} \left(\sigma^{\mathrm{S}}_{ji}\right)^{\nabla} &= C_{jikl} D^{\mathrm{e}}_{kl} \\ \left(\sigma^{\mathrm{A}}_{ji}\right)^{\nabla} &= \mu (\dot{\omega}^{\mathrm{e}}_{ij} - W^{\mathrm{e}}_{ij}) \\ \left(\tau_{kji}/\ell\right)^{\nabla} &= \mu_c \dot{\omega}^{\mathrm{e}}_{ij,k}\, \ell \end{aligned} \tag{13}$$

where C_{jikl}, μ, and μ_c are elastic material parameters and ℓ is a length scale to match the dimensions. Superposed ∇ represents the Jaumann rate of the stress measures (Mühlhaus and Vardoulakis, 1987). Superscripts e on the strain-rate measures indicate their elastic contributions.

The plastic constitutive law is also assumed to have the form of the associated flow theory with the yield function f expressed as follows:

$$f = \sqrt{3J_2} - \overline{\sigma}(\gamma) \tag{14}$$

where $\overline{\sigma}$ is the yield stress and is a function of a plastic strain invariant γ. The generalized shear stress invariant J_2 and the generalized plastic shear strain-rate invariant $\dot{\gamma}$ are defined as follows:

$$\begin{aligned} J_2 &= (a_1 + a_2) s_{ij} s_{ij} + (a_1 - a_2) \sigma^{\mathrm{A}}_{ij} \sigma^{\mathrm{A}}_{ij} + 2 a_3 \tau_{kji} \tau_{kji} / \ell^2 \\ \dot{\gamma}^2 &= (b_1 + b_2) e^{\mathrm{p}}_{ij} e^{\mathrm{p}}_{ij} + (b_1 - b_2) \left(\dot{\omega}^{\mathrm{p}}_{ij} - W^{\mathrm{p}}_{ij}\right) \left(\dot{\omega}^{\mathrm{p}}_{ij} - W^{\mathrm{p}}_{ij}\right) \\ &\quad + \frac{b_3}{2} \dot{\omega}^{\mathrm{p}}_{ij,k} \dot{\omega}^{\mathrm{p}}_{ij,k} \ell^2 \end{aligned} \tag{15}$$

The deviatoric part of the macro-stress σ^{S}_{ij} is denoted by s_{ij}. Superscripts p on the strain-rate measures indicate their plastic contributions. The deviatoric part of D^{p}_{ij} is denoted by e^{p}_{ij}. The coefficients a_1, a_2, a_3, b_1, b_2, and b_3 are determined by the requirements explained below.

The first requirement is that these invariants should be consistent with the conventional J_2-flow theory. Therefore it is required that

$$\begin{aligned} a_1+a_2&=\frac{1}{2}\\ b_1+b_2&=\frac{2}{3}\end{aligned} \tag{16}$$

The second requirement is that, in the J_2-flow theory, the plastic flow parameter $\dot{\lambda}$ should be equal to the invariant of the plastic strain-rate (de Borst, 1993). Thus,

$$\dot{\gamma}=\dot{\lambda} \tag{17}$$

This results in

$$\begin{aligned} (a_1-a_2)\left(3\left(a_1-a_2\right)\left(b_1-b_2\right)-1\right)&=0\\ a_3\left(3a_3b_3-1\right)&=0\end{aligned} \tag{18}$$

Note that if $a_1=a_2$ and $a_3=0$, this model reduces to the standard J_2-flow theory. Therefore, it is assumed that $a_1\neq a_2$ and $a_3\neq 0$ from now on. In this case, Eq. (18) can be written as follows:

$$\begin{aligned} 3\left(a_1-a_2\right)\left(b_1-b_2\right)&=1\\ 3a_3b_3&=1\end{aligned} \tag{19}$$

3 Multiscale approach for the expression of the virtual internal power

In order to apply the previously reviewed micropolar continuum to practical problems, the parameters ℓ, C_{jikl}, μ, μ_c, a_1, a_2, a_3, b_1, b_2, and b_3 in the constitutive relations need to be determined. Additional requirements are proposed by de Borst (1993) which are derived from the point of view of fast convergence in the return mapping procedure. In this paper, a multiscale approach is employed to determine some of these unknown parameters.

Define a local coordinate system z_i whose origin is located at the current position of a given macro-scale material point $\bar{\mathbf{x}}=\mathbf{x}\left(\bar{\mathbf{X}},t\right)$. Define a sub-domain of characteristic length ℓ_z surrounding $\bar{\mathbf{x}}$. This domain is called *the domain of influence* (DOI) and is denoted by Ω_z. A typical square DOI is shown in Fig. 1. Define a weight function w_z whose support is the same as Ω_z such that

$$\begin{aligned} w_z\neq 0 \quad &, z_i\in\Omega_z\\ w_z=0 \quad &, z_i\notin\Omega_z\end{aligned} \tag{20}$$

and it is normalized as

$$\int_{\Omega_z} w_z \mathrm{d}\Omega=1 \tag{21}$$

Assuming that the geometrical center of Ω_z is located at $\bar{\mathbf{x}}$, one can obtain

$$\int_{\Omega_z} w_z z_i \mathrm{d}\Omega=0 \tag{22}$$

For later use, define the second moment of the weight function as

$$B_{ij}=\int_{\Omega_z} w_z z_i z_j \mathrm{d}\Omega \tag{23}$$

For example, if the weight function is a hat function:

$$\begin{aligned} w_z=\tfrac{1}{V_z} \quad &, z_i\in\Omega_z\\ w_z=0 \quad &, z_i\notin\Omega_z\end{aligned} \tag{24}$$

where V_z is the volume of the DOI, the second moment is

$$B_{ij}=\left\{\begin{array}{ll} \frac{\ell_z^2}{12}\delta_{ij} & \text{for a 2D square DOI}\\ \frac{\ell_z^2}{16}\delta_{ij} & \text{for a 2D circular DOI}\end{array}\right\} \tag{25}$$

where δ_{ij} denotes the Kronecker delta function. For later use, define a scalar parameter B as

$$B=\left\{\begin{array}{ll} \frac{1}{12} & \text{for a 2D square DOI}\\ \frac{1}{16} & \text{for a 2D circular DOI}\end{array}\right\} \tag{26}$$

The size of the DOI ℓ_z represents the extent of influence of microstructural features, and the weight function w_z represents the intensity of the influence. Therefore, ℓ_z and w_z have to be determined by theoretical, experimental, or numerical approaches which can directly deal with the discrete microstructure. In most of the example problems of granular medium shown later, the characteristic length of densely packed soil introduced in Gaspar and Koenders (2001) is selected. That is $\ell_z=10R$ where R is the radius of the grains.

Because of the local support of the weight function, the internal power density at $\bar{\mathbf{x}}$ is only affected by the points inside the DOI. As it is shown later, the size of the DOI plays an important role in determining the deformation which occurs after failure. It should be changed according to the deformation or other state variables. Also, there should be higher order variation of velocity $\dot{u}_i$ and the micro-spin $\dot{\omega}_{ij}$ inside the DOI.

However, this paper concentrates on the simplest case in order to make the analyses clear. The size of the DOI and the weight function are kept constant over the entire domain and over the entire analysis period. Also, when the virtual internal power is evaluated, only the linear variation inside the DOI according to the relative position z_i is considered for the velocity and the micro-spin. By the assumptions above, the macro-velocity gradient L_{ij} is kept constant in the DOI and it is only a function of $\overline{\mathbf{X}}$, while the micro-spin $\dot{\omega}_{ij}$ is a function of both $\overline{\mathbf{X}}$ and $\mathbf{z}$. Let

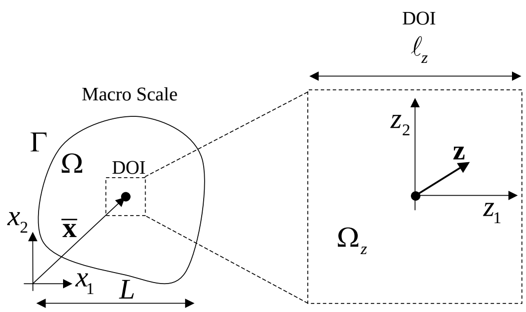

Figure 1 : A square domain of influence.

$\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)$ denote the microscopic internal power density at a point in the DOI. Expanding it in terms of $\dot{\omega}_{ij}\left(\overline{\mathbf{X}},\mathbf{z}\right)$ around $\dot{\omega}_{ij}\left(\overline{\mathbf{X}},\mathbf{z}\right)=W_{ij}\left(\overline{\mathbf{X}}\right)$ and truncating at the second order, one has

$$\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)=\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)\big|_{\dot{\omega}_{ij}=W_{ij}} +\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\left(\dot{\omega}_{ij}\left(\overline{\mathbf{X}},\mathbf{z}\right)-W_{ij}\left(\overline{\mathbf{X}}\right)\right) \tag{27}$$

where $\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)$ is defined as the gradient of the microscopic internal power density in terms of the micro-spin:

$$\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\equiv\left.\frac{\partial\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)}{\partial\dot{\omega}_{ij}}\right|_{\dot{\omega}_{ij}=W_{ij}} \tag{28}$$

Note that $\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)$ has a unit of stress, and it generates internal power with the relative spin between the micro-spin and the macro-spin.

Assume a situation where deformation in the DOI is homogeneous. In this situation, the micro-spin is equal to the macro-spin and constant everywhere in the DOI. The microscopic internal power density of this state can be expressed by the macro-stress $\sigma^{\text{S}}_{ji}\left(\overline{\mathbf{X}}\right)$ and the macro rate-of-deformation tensor $D_{ij}\left(\overline{\mathbf{X}}\right)$ as

$$\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)\big|_{\dot{\omega}_{ij}=W_{ij}}=\sigma^{\text{S}}_{ji}\left(\overline{\mathbf{X}}\right)D_{ij}\left(\overline{\mathbf{X}}\right),\ \forall\mathbf{z}\in\Omega_z \tag{29}$$

Using Eq. (29), Eq. (27) becomes

$$\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)=\sigma^{\text{S}}_{ji}\left(\overline{\mathbf{X}}\right)D_{ij}\left(\overline{\mathbf{X}}\right) +\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\left(\dot{\omega}_{ij}\left(\overline{\mathbf{X}},\mathbf{z}\right)-W_{ij}\left(\overline{\mathbf{X}}\right)\right) \tag{30}$$

The proposed method expresses the macro internal power density at a given macro-scale material point $\overline{\mathbf{X}}$ by the weighted average of the microscopic internal power density over the DOI as

$$\tilde{e}^{\text{int}}(\overline{\mathbf{X}})=\int_{\Omega_z}w_z\left(\mathbf{z}\right)\dot{e}^{\text{int}}\left(\overline{\mathbf{X}},\mathbf{z}\right)\text{d}\Omega \tag{31}$$

This operation puts the length-scale ℓ_z into the expression of the macroscopic internal power, thus non-local characteristics are included in the governing equations. Since the micro-spin is assumed to be linearly dependent on the relative position z_i, one has

$$\tilde{e}^{\text{int}}\left(\overline{\mathbf{X}}\right)=\sigma^{\text{S}}_{ji}\left(\overline{\mathbf{X}}\right)D_{ij}\left(\overline{\mathbf{X}}\right)+\sigma^{\text{A}}_{ji}\left(\overline{\mathbf{X}}\right)\left(\dot{\omega}_{ij}\left(\overline{\mathbf{X}}\right)-W_{ij}\left(\overline{\mathbf{X}}\right)\right) +\tau_{kji}\left(\overline{\mathbf{X}}\right)\dot{\omega}_{ij,k}\left(\overline{\mathbf{X}}\right) \tag{32}$$

where σ^{A}_{ji} and τ_{kji} are defined as the zeroth and the first moment of $\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)$ as follows:

$$\sigma^{\text{A}}_{ji}\left(\overline{\mathbf{X}}\right)\equiv\int_{\Omega_z}w_z(\mathbf{z})\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\text{d}\Omega \tag{33a}$$

$$\tau_{kji}\left(\overline{\mathbf{X}}\right)\equiv\int_{\Omega_z}w_z(\mathbf{z})z_k\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\text{d}\Omega \tag{33b}$$

The total internal power for the entire domain is obtained by integrating Eq. (32) over the entire domain. It gives the same expression as Eq. (3). A major difference from the past work is that this formulation derives the micro-stress and the couple stress from the moments of β_{ji}.

4 Constitutive relations for a granular material

4.1 Elastic constitutive relation

When considering the evolution of β_{ji} according to the deformation, it is natural to relate β_{ji} to the elastic portion of the difference between the micro-spin and the macro-spin so that it acts to decrease the relative spin. A simple elastic response is assumed such that

$$\left(\beta_{ji}\left(\overline{\mathbf{X}},\mathbf{z}\right)\right)^{\nabla}=\mu_c\left(\dot{\omega}^{\mathrm{e}}_{ij}\left(\overline{\mathbf{X}},\mathbf{z}\right)-W^{\mathrm{e}}_{ij}\left(\overline{\mathbf{X}}\right)\right) \tag{34}$$

where μ_c is the rotational elastic modulus which is assumed to be constant in the DOI. By the definitions in Eq. (33) and by the assumption that $\dot{\omega}_{ij}$ is linearly distributed in the DOI, one can obtain

$$\left(\sigma^{\mathrm{A}}_{ji}\left(\overline{\mathbf{X}}\right)\right)^{\nabla}=\mu_c\left(\dot{\omega}^{\mathrm{e}}_{ij}\left(\overline{\mathbf{X}}\right)-W^{\mathrm{e}}_{ij}\left(\overline{\mathbf{X}}\right)\right) \tag{35a}$$

$$\left(\tau_{kji}\left(\overline{\mathbf{X}}\right)\right)^{\nabla}=\mu_c B_{kn}\dot{\omega}^{\mathrm{e}}_{ij,n}\left(\overline{\mathbf{X}}\right) \tag{35b}$$

For the symmetric stress σ^{S}_{ji}, the conventional elastic constitutive relation is applied. In the two-dimensional plane strain condition, because of the symmetric and skew-symmetric properties of the stress measures and the strain-rate measures, one can define a generalized stress vector and a generalized strain-rate vector with the size of DOI ℓ_z as

$$\sigma=\left\{\begin{array}{c}\sigma^{\mathrm{S}}_{xx}\\ \sigma^{\mathrm{S}}_{yy}\\ \sigma^{\mathrm{S}}_{zz}\\ \sigma^{\mathrm{S}}_{xy}\\ \sigma^{\mathrm{A}}_{xy}\\ \tau_{xxy}/\ell_z\\ \tau_{yxy}/\ell_z\end{array}\right\},\ \dot{\varepsilon}=\left\{\begin{array}{c}D_{xx}\\ D_{yy}\\ 0\\ 2D_{xy}\\ 2\left(\dot{\omega}_{yx}-W_{yx}\right)\\ 2\ell_z\dot{\omega}_{yx,x}\\ 2\ell_z\dot{\omega}_{yx,y}\end{array}\right\} \tag{36}$$

With this expression, the elastic response of this material can be written as follows:

$$\boldsymbol{\sigma}^{\nabla}=\mathbf{C}\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} \tag{37}$$

where

$$\mathbf{C}=\left[\begin{array}{ccccccc}C_1&C_2&C_2&0&0&0&0\\ C_2&C_1&C_2&0&0&0&0\\ C_2&C_2&C_1&0&0&0&0\\ 0&0&0&\mu&0&0&0\\ 0&0&0&0&\mu_c&0&0\\ 0&0&0&0&0&B\mu_c&0\\ 0&0&0&0&0&0&B\mu_c\end{array}\right] \tag{38}$$

$$C_1=\frac{2\mu(1-\nu)}{1-2\nu}\ ,\ C_2=\frac{2\mu\nu}{1-2\nu} \tag{39}$$

and Poisson's ratio and the elastic shear modulus are denoted by ν and μ, respectively.

4.2 Plastic constitutive relation

The plastic constitutive relation is developed for a simple granular material model in a similar manner as the couple stress approach of Mühlhaus and Vardoulakis (1987). The generalized strain-rate invariant $\dot{\gamma}$ is expressed by the average of the inter-particle slip. The distinction of the proposed method is that $\dot{\gamma}$ is derived from the spatial averaging over the same DOI as that for the virtual internal power.

Suppose the material microstructure is represented by an aggregation of rigid circular particles of the same radius R in the plane strain condition. Let $\overline{\mathbf{x}}$, $\mathbf{z}^A$ and $\mathbf{z}^B$ denote the current position of the center of the DOI and the center of two particles, respectively (Fig. 2). The velocity of the center of these particles are denoted by $\dot{u}_i\left(\mathbf{z}^A\right)$ and $\dot{u}_i\left(\mathbf{z}^B\right)$. Assuming that the plastic contribution of the macro-velocity gradient L^{p}_{ij} is constant in the DOI, one can write

$$\begin{array}{l}\dot{u}_i\left(\mathbf{z}^A\right)=\dot{u}_i\left(\overline{\mathbf{x}}\right)+L^{\mathrm{p}}_{ij}\left(\overline{\mathbf{x}}\right)z^A_j\\ \dot{u}_i\left(\mathbf{z}^B\right)=\dot{u}_i\left(\overline{\mathbf{x}}\right)+L^{\mathrm{p}}_{ij}\left(\overline{\mathbf{x}}\right)z^B_j\end{array} \tag{40}$$

Let $\dot{u}^A_i\left(\mathbf{z}^c\right)$ and $\dot{u}^B_i\left(\mathbf{z}^c\right)$ denote the velocity at the contact

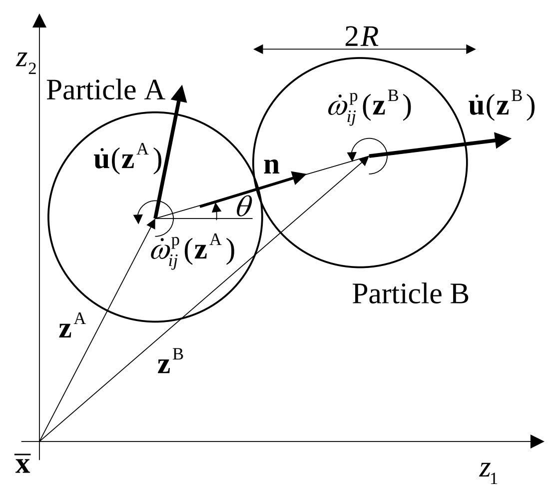

Figure 2 : Microstructure of a granular material

point on each particle, respectively, where $\mathbf{z}^c$ is the position of the contact point. Since the particles are rigid, these velocities can be written with the micro-spin $\dot{\omega}^{\mathrm{p}}_{ij}$ as follows:

$$\begin{array}{l}\dot{u}^A_i\left(\mathbf{z}^c\right)=\dot{u}_i\left(\mathbf{z}^A\right)+R\dot{\omega}^{\mathrm{p}}_{ij}\left(\mathbf{z}^A\right)n_j\\ \dot{u}^B_i\left(\mathbf{z}^c\right)=\dot{u}_i\left(\mathbf{z}^B\right)-R\dot{\omega}^{\mathrm{p}}_{ij}\left(\mathbf{z}^B\right)n_j\end{array} \tag{41}$$

where n_j denotes the unit vector normal to the contact surface. The relative velocity at the contact point $\Delta\dot{u}_i$ is

$$\begin{aligned}\Delta\dot{u}_i(\mathbf{z}^c) &= \dot{u}_i^B(\mathbf{z}^c) - \dot{u}_i^A(\mathbf{z}^c)\\ &= 2R\left(L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) - \frac{\dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}^A) + \dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}^B)}{2}\right)n_j \end{aligned} \quad (42)$$

Since the micro-spin field is assumed to be linearly distributed in a DOI and $\mathbf{z}^c = \frac{\mathbf{z}^A+\mathbf{z}^B}{2}$, one can write

$$\Delta\dot{u}_i(\mathbf{z}^c) = 2R\left(L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) - \dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}^c)\right)n_j \quad (43)$$

Let the relative velocity normal to and tangential to the contact surface be denoted by $\Delta\dot{u}_i^n(\mathbf{z}^c)$ and $\Delta\dot{u}_i^t(\mathbf{z}^c)$, respectively. They can be written as follows:

$$\begin{aligned}\Delta\dot{u}_i^n(\mathbf{z}^c) &= \Delta\dot{u}_l(\mathbf{z}^c)\,n_l n_i\\ \Delta\dot{u}_i^t(\mathbf{z}^c) &= \Delta\dot{u}_i(\mathbf{z}^c) - \Delta\dot{u}_i^n(\mathbf{z}^c)\\ &= 2Rn_j\left(L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) - \dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}^c) - L_{lj}^{\mathrm{p}}(\mathbf{z}^c)\,n_l n_i\right)\end{aligned} \quad (44)$$

Define a quantity called slip as the relative velocity tangential to the contact surface normalized by $2\pi R$. Let $s(\mathbf{z}^c,\mathbf{n})$ denote the square of the slip at a contact point located at $\mathbf{z}^c$ and whose direction of contact is n_j such that

$$\begin{aligned}s(\mathbf{z}^c,\mathbf{n}) &= \Delta\dot{u}_i^t(\mathbf{z}^c)\,\Delta\dot{u}_i^t(\mathbf{z}^c)\,(2\pi R)^{-2}\\ &= 4R^2 n_j n_s (2\pi R)^{-2}\,Q_{ij}(\bar{\mathbf{x}},\mathbf{z}^c)\,Q_{is}(\bar{\mathbf{x}},\mathbf{z}^c)\\ &\quad - 4R^2 n_j n_s (2\pi R)^{-2}\,L_{lj}^{\mathrm{p}}(\bar{\mathbf{x}})\,L_{ts}^{\mathrm{p}}(\bar{\mathbf{x}})\,n_l n_t\end{aligned} \quad (45)$$

where

$$Q_{ij}(\bar{\mathbf{x}},\mathbf{z}^c) = \left(L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) - \dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}^c)\right) \quad (46)$$

In the proposed method, $\dot{\gamma}$ is defined as the square root of the double average of $s(\mathbf{z}^c,\mathbf{n})$ in terms of the direction of n_j and over the volume of the DOI as

$$\dot{\gamma}^2 \equiv A\sum_c w_c\left(\int_0^{2\pi} w_\theta(\theta)\,s(\mathbf{z}^c,\mathbf{n})\,\mathrm{d}\theta\right) \quad (47)$$

where $w_\theta(\theta)$ is the weight function for the contact direction θ, and w_c is the weight for each contact pair. A constant A is a factor determined later. The summation about c is done over all the contact points in the DOI. When there are many particles in a DOI, one can approximate the summation by an integration as

$$\dot{\gamma}^2 = A\int_{\Omega_z} w_z(\mathbf{z})\left(\int_0^{2\pi} w_\theta(\theta)\,s(\mathbf{z},\mathbf{n})\,\mathrm{d}\theta\right)\mathrm{d}\Omega \quad (48)$$

In the two-dimensional plane strain condition, n_i can be written as

$$\begin{aligned}n_1 &= \cos(\theta)\\ n_2 &= \sin(\theta)\end{aligned} \quad (49)$$

To make the analysis simple, it is assumed that the direction of contact is distributed completely randomly. Thus a constant weight function $w_\theta = \frac{1}{2\pi}$ is employed. Using the identities:

$$\int_0^{2\pi}\frac{1}{2\pi}n_i n_j\,\mathrm{d}\theta = \frac{1}{2}\delta_{ij} \quad (50)$$

$$\int_0^{2\pi}\frac{1}{2\pi}n_i n_j n_k n_l\,\mathrm{d}\theta = \frac{1}{8}\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \quad (51)$$

Eq. (48) becomes

$$\begin{aligned}\dot{\gamma}^2 &= \frac{A}{\pi^2}\int_{\Omega_z}\frac{1}{2}Q_{ij}(\bar{\mathbf{x}},\mathbf{z}^c)\,Q_{ij}(\bar{\mathbf{x}},\mathbf{z}^c)\,w_z(\mathbf{z})\,\mathrm{d}\Omega\\ &\quad - \frac{A}{\pi^2}\int_{\Omega_z}\frac{1}{8}\left(L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) + L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})L_{ji}^{\mathrm{p}}(\bar{\mathbf{x}})\right)w_z(\mathbf{z})\,\mathrm{d}\Omega\\ &\quad - \frac{A}{\pi^2}\int_{\Omega_z}\frac{1}{8}L_{ii}^{\mathrm{p}}(\bar{\mathbf{x}})\,L_{jj}^{\mathrm{p}}(\bar{\mathbf{x}})\,w_z(\mathbf{z})\,\mathrm{d}\Omega\end{aligned} \quad (52)$$

Decompose the macro-velocity gradient into the volumetric, the deviatoric, and the skew-symmetric parts as

$$L_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) = \dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) + D^{\mathrm{pv}}(\bar{\mathbf{x}})\,\delta_{ij} + W_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) \quad (53)$$

where $\dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})$ and $D^{\mathrm{pv}}(\bar{\mathbf{x}})$ denote the deviatoric part and volumetric part of the plastic rate-of-deformation at the macro-scale. Substituting Eq. (53) into Eq. (52) yields

$$\begin{aligned}\dot{\gamma}^2 &= \frac{A}{4\pi^2}\int_{\Omega_z}\dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\,\dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\,w_z(\mathbf{z})\,\mathrm{d}\Omega\\ &\quad + \frac{A}{4\pi^2}\int_{\Omega_z}2\Delta\dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}},\mathbf{z})\,\Delta\dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}},\mathbf{z})\,w_z(\mathbf{z})\,\mathrm{d}\Omega\end{aligned} \quad (54)$$

where

$$\Delta\dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}},\mathbf{z}) = \left(\dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}) - W_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\right) \quad (55)$$

Because $\dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z})$ is linearly dependent on z_i as

$$\dot{\omega}_{ij}^{\mathrm{p}}(\mathbf{z}) = \dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) + \dot{\omega}_{ij,k}^{\mathrm{p}}(\bar{\mathbf{x}})\,z_k \quad (56)$$

and a constant weight function $\frac{1}{V_z}$ is assumed for $w_z(\mathbf{z})$, substituting Eq. (56) into Eq. (54) yields

$$\begin{aligned}\dot{\gamma}^2 &= \frac{A}{4\pi^2 V_z}\int_{\Omega_z}\dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\,\dot{e}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}}) + 2\Delta\dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\,\Delta\dot{\omega}_{ij}^{\mathrm{p}}(\bar{\mathbf{x}})\,\mathrm{d}\Omega\\ &\quad + \frac{A}{4\pi^2 V_z}\int_{\Omega_z}\left(2\dot{\omega}_{ij,k}(\bar{\mathbf{x}})\,\dot{\omega}_{ij,l}(\bar{\mathbf{x}})\,z_k z_l\right)\mathrm{d}\Omega\end{aligned} \quad (57)$$

Using Eq. (22) and the definition of B_{ij} in Eq. (23), one can obtain

$$\dot{\gamma}^2 = \frac{A}{4\pi^2}\dot{e}^{\mathrm{p}}_{ij}(\bar{\mathbf{x}})\,\dot{e}^{\mathrm{p}}_{ij}(\bar{\mathbf{x}}) + \frac{A}{4\pi^2}\left(2\Delta\dot{\omega}^{\mathrm{p}}_{ij}(\bar{\mathbf{x}})\,\Delta\dot{\omega}^{\mathrm{p}}_{ij}(\bar{\mathbf{x}}) + 2B_{lk}\dot{\omega}^{\mathrm{p}}_{ij,k}(\bar{\mathbf{x}})\,\dot{\omega}^{\mathrm{p}}_{ij,l}(\bar{\mathbf{x}})\right) \tag{58}$$

In order to coincide with the shear strain-rate invariant of the conventional continuum, A is chosen as $\frac{8\pi^2}{3}$. The final form for the shear strain-rate invariant is

$$\dot{\gamma} = \sqrt{\frac{2}{3}\dot{e}^{\mathrm{p}}_{ij}\dot{e}^{\mathrm{p}}_{ij} + \frac{4}{3}\Delta\dot{\omega}^{\mathrm{p}}_{ij}\Delta\dot{\omega}^{\mathrm{p}}_{ij} + \frac{4B_{lk}}{3}\dot{\omega}^{\mathrm{p}}_{ij,k}\dot{\omega}^{\mathrm{p}}_{ij,l}} \tag{59}$$

where the argument $\bar{\mathbf{x}}$ is omitted since all the terms are a function of $\bar{\mathbf{x}}$ only. Since the length scale ℓ is defined as $\ell = \ell_z$ in the previous sub-section, comparing Eq. (59) to Eq. (15) yields

$$b_1 = 1,\quad b_2 = -\frac{1}{3},\quad b_3 = \frac{8B}{3} \tag{60}$$

The parameters a_1, a_2, and a_3 are determined by the requirements in Eq. (16) and Eq. (19) as follows:

$$a_1 = \frac{3}{8},\quad a_2 = \frac{1}{8},\quad a_3 = \frac{1}{8B} \tag{61}$$

5 Numerical examples

The weak form governing equations Eq. (10) are discretized by the FEM in the one-dimensional pure shear condition and in the two-dimensional plane strain condition. The finite element formulation for the micro polar material of de Borst (1993) is employed. The discretized momentum equation is solved with the proposed constitutive relation by the central-difference explicit time-integration method (e.g. section 6.2 in (Belytschko, Liu, and Moran, 2000)) and the semi-implicit stress update method of Moran, Ortiz, and Shih (1990).

For two-dimensional examples, the bridging scale method for the micropolar continuum (Kadowaki and Liu, 2004) is employed to enhance the efficiency. This method first discretizes the entire domain by a finite element mesh which is coarse enough to complete the computation at an affordable cost. Additionally, another fine element mesh, which is fine enough to capture localized deformation in the shear bands, is utilized. This fine mesh is defined only around the localized region. Finite element computations are operated with these two meshes simultaneously interacting each other. Since the improvement of computational efficiency is out of the scope of this paper, explanation of the detailed formulation for this method is avoided.

5.1 *One-dimensional shear localization problem*

A one-dimensional shear localization problem is solved with the micropolar continuum with the proposed material parameters. A horizontal bar of length 0.2 m is sheared by the prescribed impact velocity in the y direction $u_{0y} = \pm 0.9\,\mathrm{m/s}$ at both ends. The problem statement is shown in Fig. 3. In this calculation, displacement in the x direction is constrained to zero over the entire domain. At both ends of the bar, the boundary condition $\omega_{yx} = 0$ is applied. On the top and the bottom boundary, periodic boundary conditions are applied.

Material parameters used in this calculation are: Young's modulus $E = 60.0\,\mathrm{MPa}$, $\nu = 0.45$, $\mu_c = 4.00\,\mathrm{MPa}$, and $\rho = 2.00\times 10^3\,\mathrm{kg/m^3}$. The radius of a grain is set as $R = 0.4\times 10^{-3}\,\mathrm{m}$. The length scale of the DOI is set as $\ell_z = 10R$. The inertia of micro-rotation and the initial yield stress are set as $\rho I = \rho\ell_z^2/300$ and $\bar{\sigma}_0 = 600\,\mathrm{kPa}$, respectively. Note that to avoid the restriction of time step size due to the inertia of micro-spin, the rotational inertia is set larger than the theoretical value written in the appendix. The yield stress decreases with the generalized plastic shear strain invariant γ.

In the x direction the domain is uniformly discretized by various numbers of elements, whereas there is only one element in the y direction. For this calculation, the material parameters derived by a square DOI are employed. Those are: $a_1 = \frac{3}{8}$, $a_2 = \frac{1}{8}$, $a_3 = \frac{3}{2}$, $b_1 = 1$, $b_2 = -\frac{1}{3}$, and $b_3 = \frac{2}{9}$. Fig. 4 shows the distribution of the generalized plastic shear strain invariant γ which is obtained at 0.002 seconds. As the mesh is refined, the width of the shear band and the strain distribution inside it converge to one solution. The thickness of the shear band is around ten times the diameter of the particle.

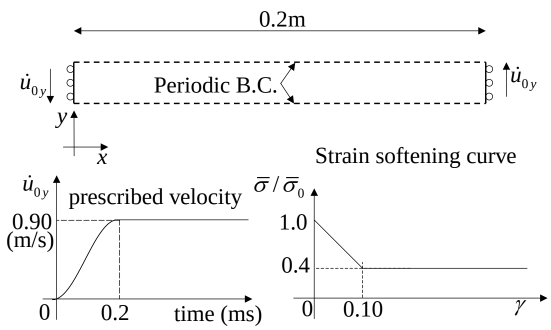

Figure 3 : One-dimensional shear localization problem.

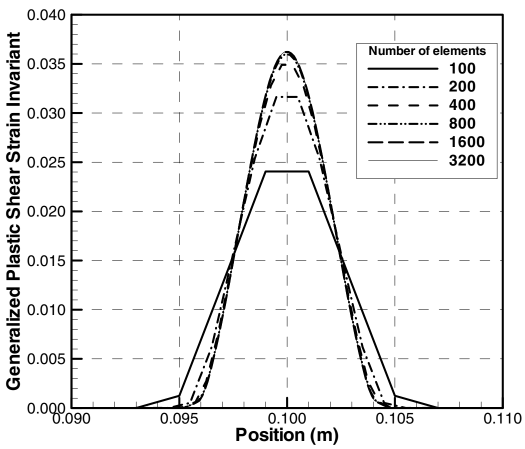

Figure 4 : Convergence test with a one-dimensional shear localization problem.

5.2 *Comparison to the existing material models*

The example problem presented in the previous subsection is analyzed with existing material models. In Tab. 1, plastic parameters proposed in this study and those proposed by de Borst (1993) and Vardoulakis (1989) are shown. Other material parameters are the same as the previous example. Although the length scale which is used in the invariants J_2 and $\dot{\gamma}$ is equal to R in the model of Vardoulakis (1989), it is replaced by $10R$ in this example in order to compare the effect of the plastic parameters. The effect of the length scale is examined in section 5.4. In Fig. 5, the generalized plastic shear strain invariant γ inside the shear-band is plotted for these three sets of material parameters. The proposed material parameters yield almost the same shear-band width, but it has a sharper strain profile inside the shear-band.

Table 1 : Comparison of the material parameters.

	a_1	a_2	a_3	b_1	b_2	b_3
Proposed	3/8	1/8	3/2	1	−1/3	2/9
Vardoulakis 1989	3/8	1/8	1/4	3	−1	4
De Borst 1993	1/4	1/4	1/2	1/3	1/3	2/3

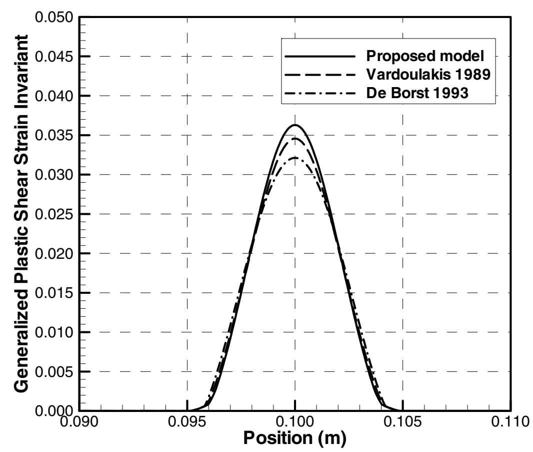

Figure 5 : Comparison to the existing models.

5.3 *Two-dimensional shear localization problem*

Two-dimensional compression examples are computed in the plane strain condition with the conventional continuum model and the micropolar continuum model with the proposed material parameters. The length of the bar is 0.4m and the width is 0.04 m (Fig. 6). Impact compressive velocity conditions are applied at both ends of the bar. Material parameters are the same as the one-dimensional example in section 5.1. Because very fine discretization is required to capture the shear-localization, the entire domain is first discretized by 8 × 80 coarse FEM elements. In addition, a fine FEM mesh is attached on the central portion and these two sets of FEM computations are coupled by the bridging scale method (Wagner and Liu, 2003; Wagner, Karpov, and Liu, 2004; Karpov, Wagner, and Liu, 2005; Kadowaki and Liu, 2004). Both the coarse-scale FEM and fine-scale FEM run simultaneously interacting with each other. Three fine FEM meshes with various numbers of elements are prepared and they are named mesh A, B, and C. Representative element sizes of mesh A, B, and C are 2.0×10^{-3} m, 1.0×10^{-3} m, and 0.5×10^{-3} m, respectively. Fig. 7 shows the coarse-scale mesh and the fine-scale mesh, A. Fig. 8 to Fig. 13 show the distribution of the generalized plastic shear strain invariant after 0.003 seconds in the fine-scale meshes. The lines of the elemet boundary are ommited for the mesh C (Fig. 10 and Fig. 13), since the elements are too small to be shown in the figures. The micropolar continuum with the proposed material parameters yields almost the same result with mesh B and C, whereas the deformation is significantly affected by the size of the element with the conventional continuum model.

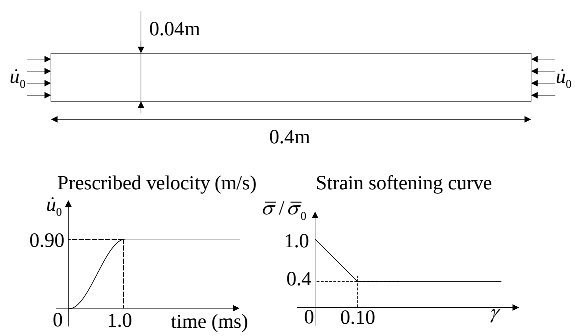

Figure 6 : Two-dimensional shear localization problem.

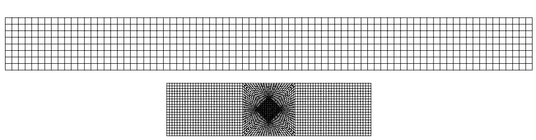

Figure 7 : The coarse-scale mesh and the fine-scale mesh A.

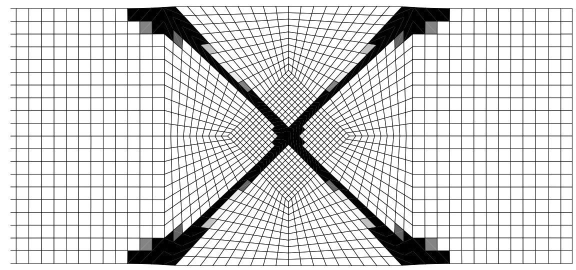

Figure 8 : Conventional continuum with mesh A.

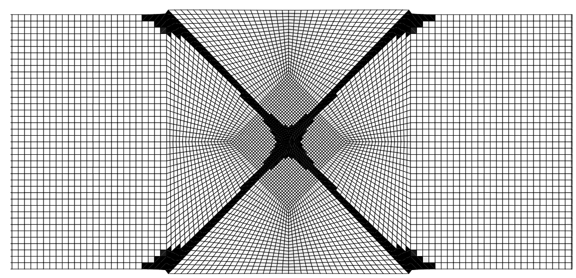

Figure 9 : Conventional continuum with mesh B.

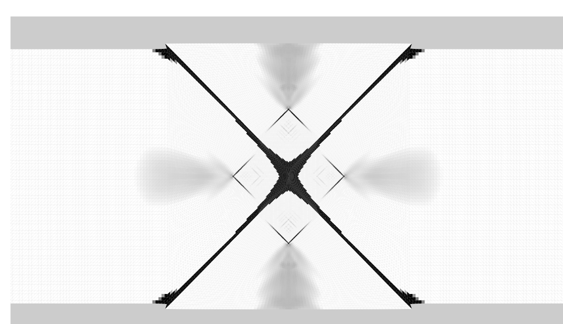

Figure 10 : Conventional continuum with mesh C.

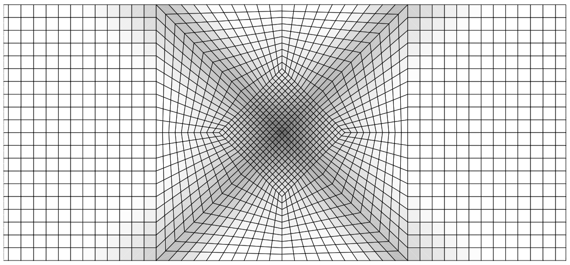

Figure 11 : Micropolar continuum with the proposed material parameters with mesh A.

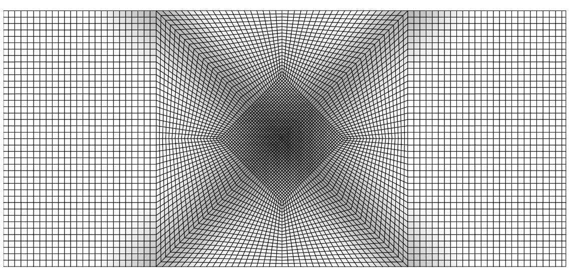

Figure 12 : Micropolar continuum with the proposed material parameters with mesh B.

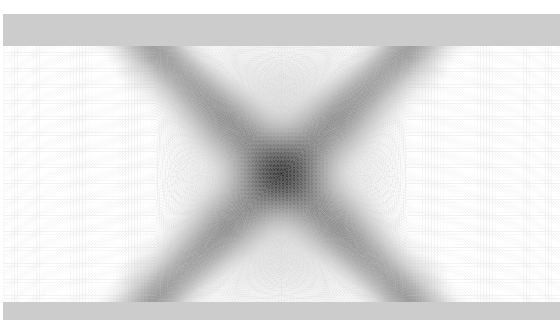

Figure 13 : Micropolar continuum with the proposed material parameters with mesh C.

5.4 *Effect of the size of DOI*

The effect of the size of the DOI is examined in this subsection. The simulated problems are the same as that of the micropolar continuum model with the proposed material parameters with mesh C in section 5.3. However, three different sizes of DOI are compared. Those are $\ell_z = 2R$, $5R$, and $20R$. Fig. 14, Fig. 15, and Fig. 16 show the generalized plastic shear strain invariant after the failure. Comparing to Fig. 13 $(\ell_z = 10R)$, it is clear that the size of the DOI affects the results significantly. Smaller DOI results in narrower and sharper shear bands.

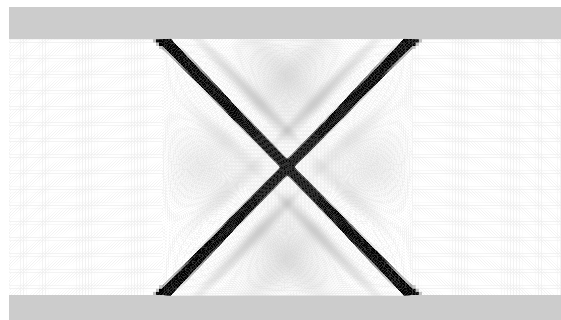

Figure 14 : Generalized plastic shear strain invariant profile for $\ell_z = 2R$

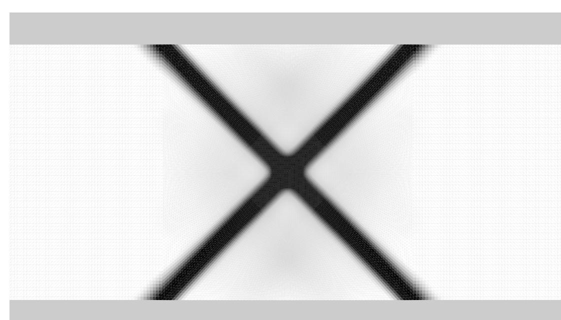

Figure 15 : Generalized plastic shear strain invariant profile for $\ell_z = 5R$

6 Conclusions

A multiscale approach to derive material parameters for the micropolar continuum model is proposed. The parameters are determined considering the microstructure

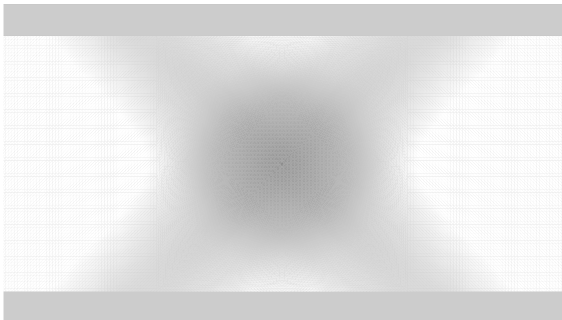

Figure 16 : Generalized plastic shear strain invariant profile for $\ell_z = 20R$

through averaging operations over the DOI. The length scale in the governing equation and the constitutive relations is defined as the size of the DOI, i.e. the extent of the interaction within the microstructure. This concept can at least limit the arbitrariness of this parameter. The elastic modulus for the couple stress is obtained by averaging the internal power over the DOI. Plastic parameters are determined through averaging inter-particle slip among the microstructure. The proposed model yields similar results as the existing couple stress models and successfully regularizes the solution for failure phenomena of a strain-softening rate-independent material.

Limitations of this study are listed below and further studies are expected for them.

- Evolution law for the DOI should be incorporated.
- The effects of higher order variation of velocity and micro-spin inside the DOI should be examined.
- There is still arbitrariness for the elastic constant μ_c and the length scale ℓ_z. This study can limit the order of ℓ_z to the same order of the characteristic length of the microstructure, but can not exactly determine it.
- Volumetric plastic deformation should be included in the model for both macro-material model and micro-material model.

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References

Bažant, Z. P.; Belytschko, T. B. (1985): Wave-propagation in a strain-softening bar - exact solution. *Journal of Engineering Mechanics-Asce*, vol. 111, no. 3, pp. 381–389.

Bažant, Z. P.; Belytschko, T. B.; Chang, T. P. (1984): Continuum theory for strain-softening. *Journal of Engineering Mechanics-Asce*, vol. 110, no. 12, pp. 1666–1692.

Belytschko, T.; Liu, W. K.; Moran, B. (2000): *Nonlinear Finite Elements for Continua and Structures*. John Wiley, Chichester ; New York.

Chen, Y.; Lee, D. J.; Eskandarian, A. (2004): Micropolar theory and its applicatins to mesoscopic and microscopic problems. *CMES: Computer Modeling in Engineering & Scineces*, vol. 5, no. 1, pp. 35–43.

de Borst, R. (1993): A generalization of J_2-flow theory for polar continua. *Computer Methods in Applied Mechanics and Engineering*, vol. 103, no. 3, pp. 347–362.

de Borst, R.; Sluys, L. J.; Mühlhaus, H.; Pamin, J. (1993): Fundamental issues in finite element analyses of localization of deformation. *Engineering Computations*, vol. 10, pp. 99–121.

Eringen, A. C.; Suhubi, E. S. (1964): Nonlinear theory of simple micro-elastic solids. *International Journal of Engineering Science*, vol. 2, pp. 189–203.

Gao, H.; Huang, Y.; Nix, W. D.; Hutchinson, J. W. (1999): Mechanism-based strain gradient plasticity - I. theory. *Journal of the Mechanics and Physics of Solids*, vol. 47, no. 6, pp. 1239–1263.

Gaspar, N.; Koenders, M. A. (2001): Micromechanic formulation of macroscopic structures in a granular medium. *Journal of Engineering Mechanics*, vol. 127, no. 10, pp. 987–993.

Germain, P. (1973): Method of virtual power in continuum mechanics .2. microstructure. *Siam Journal on Applied Mathematics*, vol. 25, no. 3, pp. 556–575.

Kadowaki, H.; Liu, W. K. (2004): Bridging multi-scale method for localization problems. *Computer Methods in Applied Mechanics and Engineering*, vol. 193, pp. 3267–3302.

Karpov, E. G.; Stephen, N. G.; Dorofeev, D. L. (2002): On static analysis of finite repetitive structures by discrete Fourier transform. *International Journal of Solids and Structures*, vol. 39, no. 16, pp. 4291–4310.

Karpov, E. G.; Stephen, N. G.; Liu, W. K. (2003): Initial tension in randomly disordered periodic lattices. *International Journal of Solids and Structures*, vol. 40, no. 20, pp. 5371–5388.

Karpov, E. G.; Wagner, G. J.; Liu, W. K. (2005): A Green's function approach to deriving non-reflecting boundary conditions in molecular dynamics simulations. *International Journal for Numerical Methods in Engineering*, vol. 62, no. 9, pp. 1250-1262.

Kouznetsova, V.; Geers, M. G. D.; Brekelmans, W. A. M. (2002): Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. *International Journal for Numerical Methods in Engineering*, vol. 54, pp. 1235–1260.

Lasry, D.; Belytschko, T. (1988): Localization limiters in transient problems. *International Journal of Solids and Structures*, vol. 24, no. 6, pp. 581–597.

Liu, W. K.; Karpov, E. G.; Zhang, S.; Park, H. S. (2004): An introduction to computational nano mechanics and materials. *Computer Methods in Applied Mechanics and Engineering*, vol. 193, pp. 1529–1578.

Liu, W. K.; Uras, R. A.; Chen, Y. (1997): Enrichment of the finite element method with the reproducing kernel particle method. *Journal of Applied Mechanics-Transactions of the Asme*, vol. 64, no. 4, pp. 861–870.

Moran, B.; Ortiz, M.; Shih, C. F. (1990): Formulation of implicit finite-element methods for multiplicative finite deformation plasticity. *International Journal for Numerical Methods in Engineering*, vol. 29, no. 3, pp. 483–514.

Mühlhaus, H. B.; Vardoulakis, I. (1987): The thickness of shear bands in granular materials. *Geotechnique*, vol. 37, no. 3, pp. 271–283.

Needleman, A. (1988): Material rate dependence and mesh sensitivity in localization problems. *Computer Methods in Applied Mechanics and Engineering*, vol. 67, no. 1, pp. 69–85.

Park, H. S.; Karpov, E. G.; Liu, W. K.; Klein, P. A. (2004): The bridging scale for two-dimensional atomistic/continuum coupling. *Philosophical Magazine*, vol. 85, no. 1, pp. 79-113.

Park, H. S.; Liu, W. K. (2004): An introduction and tutorial on multiple-scale analysis in solids. *Computer Methods in Applied Mechanics and Engineering*, vol. 193, pp. 1733–1772.

Vardoulakis, I. (1989): Shear-banding and liquefaction in granular-materials on the basis of a Cosserat continuum theory. *Ingenieur Archiv*, vol. 59, no. 2, pp. 106–113.

Wagner, G. J.; Karpov, E. G.; Liu, W. K. (2004): Molecular dynamics boundary conditions for regular crystal lattices. *Computer Methods in Applied Mechanics and Engineering*, vol. 193, pp. 1579–1601.

Wagner, G. J.; Liu, W. K. (2003): Coupling of atomistic and continuum simulations using a bridging scale decomposition. *Journal of Computational Physics*, vol. 190, pp. 249–274.

Appendix A: The virtual kinetic power

In this paper, the virtual kinetic power is derived in a similar manner as Germain (1973). Consider a rigid particle translating with the velocity $\dot{u}_i$ and rotating with the micro-spin $\dot{\omega}_{ij}$. Let y_i denote the position of a micro-scale material point on the particle relative to the mass center of the particle. The total velocity of this material point $\dot{u}'_i$ is expressed by

$$\dot{u}'_i = \dot{u}_i + \dot{\omega}_{ij} y_j \tag{62}$$

Let ρ' denote the microscopic mass density. The mass of a particle m is

$$m = \int_{\Omega_y} \rho' \mathrm{d}\Omega \tag{63}$$

where Ω_y is the domain of the particle. Note that m is a constant with respect to time. For later use, define I_{ij} as

$$I_{ij} = \frac{1}{m} \int_{\Omega_y} \rho' y_i y_j \mathrm{d}\Omega \tag{64}$$

The virtual kinetic power of this particle δp^{kin} is defined as

$$\begin{aligned}\delta p^{\mathrm{kin}} &= \int_{\Omega_y} \rho' \ddot{u}'_i \delta \dot{u}'_i \mathrm{d}\Omega \\ &= \int_{\Omega_y} \rho' \left(\ddot{u}_i + \ddot{\omega}_{ij} y_j + \dot{\omega}_{ip} \dot{\omega}_{pj} y_j\right) \left(\delta \dot{u}_i + \delta \dot{\omega}_{ik} y_k\right) \mathrm{d}\Omega\end{aligned} \tag{65}$$

Since the origin of the local coordinate y_i is located at the mass center of the particle

$$\int_{\Omega_y} \rho' y_i \mathrm{d}\Omega = 0 \tag{66}$$

Also, because of the skew-symmetric property of $\dot{\omega}_{ij}$

$$\dot{\omega}_{ip}\dot{\omega}_{pj}\delta\dot{\omega}_{ik} = 0 \tag{67}$$

Using these properties, one can obtain

$$\delta p^{\mathrm{kin}} = m\ddot{u}_i\delta\dot{u}_i + mI_{jk}\ddot{\omega}_{ij}\delta\dot{\omega}_{ik} \tag{68}$$

In order to derive the continuum expression of the virtual kinetic power, consider an aggregation of identical particles and a point among them. Let a small volume around this point be denoted by ΔV. The macro density ρ of this point is defined as

$$\rho = \frac{\sum^{c} m}{\Delta V}$$

where c is the number of particles included in ΔV. Note that ΔV should be smaller than the DOI so that one can neglect the variation of velocity and micro-spin inside it. Similarly, the continuum expression of the virtual kinetic power $\delta\dot{e}^{\mathrm{kin}}$ is defined as

$$\begin{aligned}\delta\dot{e}^{\mathrm{kin}} &= \frac{\sum^{c}\delta p_c^{\mathrm{kin}}}{\Delta V} \\ &= \rho\ddot{u}_i\delta\dot{u}_i + \rho I_{jk}\ddot{\omega}_{ij}\delta\dot{\omega}_{ik}\end{aligned} \tag{69}$$

where $\delta p_c^{\mathrm{kin}}$ is the virtual kinetic power of each particle included in ΔV. The macro virtual kinetic power can be obtained by integrating $\delta\dot{e}^{\mathrm{kin}}$ over the entire domain as

$$\delta P^{\mathrm{kin}} = \int_{\Omega} \rho\ddot{u}_i\delta\dot{u}_i + \rho I_{jk}\ddot{\omega}_{ij}\delta\dot{\omega}_{ik}\mathrm{d}\Omega \tag{70}$$

When the particle is assumed to be a circular disk in the plane-strain condition, one can write

$$I_{ij} = I\delta_{ij} \tag{71}$$

Therefore, one can obtain

$$\delta P^{\mathrm{kin}} = \int_{\Omega} \rho\ddot{u}_i\delta\dot{u}_i + \rho I\ddot{\omega}_{ij}\delta\dot{\omega}_{ij}\mathrm{d}\Omega \tag{72}$$