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COUPLING PARTICLE TO CONTINUUM REGIONS OF PARTICULATE MATERIALS

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ABSTRACT

Following atomistic-continuum coupling methods for lattice-structured materials [1, 2], a method for coupling particle to continuum regions of particulate materials is presented. The particle region is modeled using particle mechanics and the discrete element method, whereas the continuum region is modeled using linear micropolar elasticity and the finite element method. The formulation for coupling particle and continuum degrees of freedom as well as partitioning kinetic and potential energies in the overlapping domain is presented. Details of the numerical implementation and numerical examples will follow in a forthcoming paper. The method is developed to model particulate materials at their physical length scale (particle size) in regions of large relative particle motion in a computationally tractable manner.

INTRODUCTION

Dense, dry particulate materials are commonly found in nature and in industrial processes. Examples of such particulate materials include metallic powders (for powder metallurgy), pharmaceutical pills, agricultural grains (in silo flows), dry soils (sand, silt, gravel), and lunar and martian regolith (soil found on the surface of the Moon and Mars), for instance.

Despite their ubiquity and the associated intense efforts to understand and predict—via theoretical and numerical models—their deformation and flow behavior, particulate materials remain an unmastered class of materials with regard to modeling their spectrum of mechanical behavior in a physically-based manner across several orders of magnitude in length-scale. Particulate materials may transition in an instant from deforming like a solid to flowing like a fluid or gas and vice versa. Examples of such physical transition are the flow of metal particles generating a shear band in a metallic powder during compaction in a die, flow of quartz grains around and at the tip of a driven steel pile or earth penetrator weapon penetrating sand, the shoveling of sand by a tractor, and the flow of agricultural grains from the bulk top region through the bottom chute in a silo, for instance. These examples each involve material regions where relative neighbor particle motion is 'large' (flowing like a fluid or gas) and regions where relative neighbor particle motion is 'small' (deforming like a solid). Part of the reason for not being able to model the spectrum in a physically-based manner within one computational framework is that the length scale of the application usually is much larger than the length scale (diameter or length) of the particles composing the particulate material: 1) 50 micrometer diameter metallic particle of a metallic powder compressed in a 5 centimeter diameter die, leading to 3 orders of magnitude difference in length scale (requiring $\approx 10^9$ particles); or 2) 100 micrometer diameter quartz particle of a sand sheared by a 10 centimeter diameter earth penetrator penetrating a 1 meter deep target, which is 4 orders of magnitude difference in scale (requiring $\approx 10^{12}$ particles). As a result, it is not feasible to simulate computationally the heterogeneous, localized deformation, and flow response in the engineering application of interest involving particulate materials using a pure particle-based materials modeling approach (such as Discrete Element (DE) simulation). Hence, one solution is to develop a coupled/bridging multiscale modeling approach that models the material as discrete particles in regions where there is large relative particle motion, and as a solid continuum in regions of small relative particle motion. The challenge is how to couple these regions properly from a computational mechanics perspective and how to allow one region to transition to the other—and vice versa—through the bridging mechanics, while all done adaptively within a computational framework. This paper focusses on a method for coupling particle and continuum regions of a particulate material, presenting only the formulation for now. The numerical implementation and examples, bridging scale mechanics, and adaptivity will be addressed in future papers.

SUMMARY OF PARTICLE AND CONTINUUM REPRESENTATIONS

The balance of linear and angular momentum equations are presented for particle and continuum representations of dense, dry particulate materials. The linear micropolar elastic continuum representation is appropriate only for glued, stiff, elastic particles. A strategy for coupling these equations within an overlap region (cf. Fig.1) is summarized in the next section on COUPLING METHOD.

Particle Mechanics and Discrete Element Method

The balance of linear and angular momentum for a system of semi-rigid particles in contact may be written as [3]

$$
\begin{aligned}
&\boldsymbol{M}^Q\ddot{\boldsymbol{Q}} + \boldsymbol{C}^Q\dot{\boldsymbol{Q}} + \boldsymbol{F}^{INT,Q}(\boldsymbol{Q}) = \boldsymbol{F}^{EXT,Q} \\
&\boldsymbol{M}^Q = \mathop{\mathbf{A}}_{\delta=1}^{N} \boldsymbol{m}_\delta^Q \; ; \quad \boldsymbol{m}_\delta^Q = \begin{bmatrix} \boldsymbol{m}_\delta & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_\delta \end{bmatrix} \\
&\boldsymbol{F}^{INT,Q} = \mathop{\mathbf{A}}_{\delta=1}^{N} \boldsymbol{f}_\delta^{INT,Q} \; ; \quad \boldsymbol{f}_\delta^{INT,Q} = \sum_{\epsilon=1}^{n_c} \begin{bmatrix} \boldsymbol{f}^{\epsilon,\delta} \\ \boldsymbol{\ell}^{\epsilon,\delta} \times \boldsymbol{f}^{\epsilon,\delta} \end{bmatrix}
\end{aligned} \tag{1}
$$

where $\boldsymbol{M}^Q$ is the mass and rotary inertia matrix for a system of N particles, $\boldsymbol{m}_\delta^Q$ is the mass and rotary inertia matrix for particle δ, $\boldsymbol{m}_\delta$ is the mass matrix for particle δ, $\boldsymbol{I}_\delta$ is the rotary inertia matrix for particle δ, $\boldsymbol{C}^Q = a\boldsymbol{M}^Q$ the mass and rotary inertia proportional damping matrix with proportionality constant a (used in a dynamic relaxation solution method for quasi-static problems, but otherwise set to zero), $\boldsymbol{F}^{INT,Q}$ the internal force and moment vector associated with n_c particle contacts which is a nonlinear function of particle displacements and rotations when particles slide with friction, $\boldsymbol{f}_\delta^{INT,Q}$ the internal force and moment vector for particle δ, $\boldsymbol{f}^{\epsilon,\delta}$ the internal force vector for particle δ at contact ϵ, $\boldsymbol{\ell}^{\epsilon,\delta} \times \boldsymbol{f}^{\epsilon,\delta}$ the internal moment vector for particle δ at contact ϵ with branch vector $\boldsymbol{\ell}^{\epsilon,\delta}$, and $\boldsymbol{F}^{EXT,Q}$ the external force and moment vector. $\boldsymbol{Q}$ is the generalized degree of freedom vector for particle displacements and rotations

$$
\boldsymbol{Q} = [\boldsymbol{q}_\delta, \boldsymbol{q}_\epsilon, \ldots, \boldsymbol{q}_\eta, \boldsymbol{\theta}_\delta, \boldsymbol{\theta}_\epsilon, \ldots, \boldsymbol{\theta}_\eta]^T \; , \quad \delta, \epsilon, \ldots, \eta \in \mathcal{A} \tag{2}
$$

where $\boldsymbol{q}_\delta$ is the displacement vector of particle δ, $\boldsymbol{\theta}_\delta$ its rotation vector, and $\mathcal{A}$ is the set of free particles[1]. In general, a superscript Q denotes a variable associated with particle motion, whereas a superscript D will denote a variable associated with continuum deformation. Further details of assembling the matrices and vectors in Eq.(1) from the individual particle and particle contact contributions are not given here, as they are well established in the literature, and because this paper focusses on the coupling of the particle and continuum mechanics in an overlap region.

With regard to putting the particle mechanics and discrete element implementation into a form amenable to energy partitioning in the coupled particle-continuum overlap region, we consider an energy formulation of the balance equations using Lagrange's equation of motion. It may be stated as

$$
\frac{d}{dt}\left(\frac{\partial T^Q}{\partial \dot{\boldsymbol{Q}}}\right) - \frac{\partial T^Q}{\partial \boldsymbol{Q}} + \frac{\partial F^Q}{\partial \dot{\boldsymbol{Q}}} + \frac{\partial U^Q}{\partial \boldsymbol{Q}} = \boldsymbol{F}^{EXT,Q} \tag{3}
$$

where T^Q is the kinetic energy, F^Q the dissipation function, and U^Q the potential energy, such that

$$
T^Q = \frac{1}{2}\dot{\boldsymbol{Q}}\boldsymbol{M}^Q\dot{\boldsymbol{Q}} \tag{4}
$$

$$
F^Q = aT^Q \tag{5}
$$

$$
U^Q(\boldsymbol{Q}) = \int_{\boldsymbol{0}}^{\boldsymbol{Q}} \boldsymbol{F}^{INT,Q}(\boldsymbol{S})d\boldsymbol{S} \tag{6}
$$

The dissipation function F^Q is written as a linear function of the kinetic energy T^Q, which falls within the class of damping called Rayleigh damping, page 130 of [4]. Carrying out the derivation in Eq.(3), and using the Second Fundamental Theorem of Calculus for $\partial U^Q/\partial \boldsymbol{Q}$, leads to Eq.(1).

Micropolar Continuum and Finite Element Method

Following the formulation of Eringen [5], we present the balance of linear and angular momentum equations and finite element formulation for a linear micropolar theory of elasticity. For clarity of presentation, index tensor notation is used. The balance equations for linear and angular momentum may be written as

$$
\begin{aligned}
\sigma_{lk,l} + \rho b_k - \rho \dot{v}_k &= 0 \\
m_{lk,l} + \epsilon_{kmn}\sigma_{mn} + \rho \ell_k - \rho \dot{\beta}_k &= 0
\end{aligned} \tag{7}
$$

where σ_{lk} is the unsymmetric Cauchy stress tensor, ρ is the mass density, b_k is a body force per unit mass, v_k is the spatial velocity vector, m_{lk} is the unsymmetric couple stress, ϵ_{kmn} is the permutation operator, ℓ_k is the body couple per unit mass, β_k is the intrinsic spin per unit mass, indices $k, l, \cdots = 1, 2, 3$, and $(\bullet)_{,l} = \partial(\bullet)/\partial x_l$ denotes partial differentiation with respect to

[1] The notion of free and ghost particles will be described in the Section on COUPLING METHOD.

the spatial coordinate x_l. The intrinsic spin per unit mass is defined as

$$\beta_k \equiv j_{lk}\nu_l \quad (8)$$
$$j_{lk} \equiv i_{mm}\delta_{lk} - i_{lk} \quad (9)$$

where i_{lk} is the microinertia tensor, and δ_{lk} the Kronecker delta. The microgyration vector ν_l for the linear theory is written as

$$\nu_l = \dot{\varphi}_l \quad (10)$$

where φ_l is the microrotation vector.

Introducing w_k and η_k as weighting functions for the macrodisplacement vector u_k and microrotation vector φ_k, respectively, we apply the Method of Weighted Residuals to formulate the partial differential equations in Eq.(7) into weak form [6]. The weak, or variational, equations then result as

$$\begin{aligned} &\int_{\mathcal{B}} \rho w_k \dot{v}_k dv + \int_{\mathcal{B}} w_{k,l}\sigma_{lk} dv \\ &= \int_{\mathcal{B}} \rho w_k b_k dv + \int_{\Gamma_t} w_k t_k da \\ &\int_{\mathcal{B}} \rho \eta_k \dot{\beta}_k dv + \int_{\mathcal{B}} \eta_{k,l} m_{lk} dv - \int_{\mathcal{B}} \eta_k \epsilon_{kmn}\sigma_{mn} dv \\ &= \int_{\mathcal{B}} \rho \eta_k \ell_k dv + \int_{\Gamma_r} \eta_k r_k da \end{aligned} \quad (11)$$

where $\mathcal{B}$ is the volume of the continuum body, $t_k = \sigma_{lk}n_l$ is the applied traction on the portion of the boundary Γ_t with outward normal vector n_l, and $r_k = m_{lk}n_l$ is the applied surface couple on the portion of the boundary Γ_r.

The weak equations (11) may be approximated in Galerkin form [6], whereby the discretization parameter h implies a discrete approximation. Introducing shape functions N_a^u and N_b^φ for the macrodisplacement u_k^h and microrotation φ_k^h vectors, respectively, and assuming the microinertia is constant (j_{lk} is constant), we may write the approximations and derivatives as

$$u_k^h = \sum_{a=1}^{n_{en}^u} N_a^u d_{k(a)} \quad (12)$$
$$\dot{v}_k^h = \sum_{a=1}^{n_{en}^u} N_a^u \ddot{d}_{k(a)} \quad (13)$$
$$w_k^h = \sum_{a=1}^{n_{en}^u} N_a^u c_{k(a)} \quad (14)$$
$$w_{k,l}^h = \sum_{a=1}^{n_{en}^u} (N_a^u)_{,l} c_{k(a)} \quad (15)$$
$$\varphi_l^h = \sum_{b=1}^{n_{en}^\varphi} N_b^\varphi \phi_{l(b)} \quad (16)$$
$$\dot{\beta}_k^h = j_{lk}\ddot{\varphi}_l^h$$
$$\ddot{\varphi}_l^h = \sum_{b=1}^{n_{en}^\varphi} N_b^\varphi \ddot{\phi}_{l(b)} \quad (17)$$
$$\eta_k^h = \sum_{b=1}^{n_{en}^\varphi} N_b^\varphi g_{k(b)} \quad (18)$$
$$\eta_{k,l}^h = \sum_{b=1}^{n_{en}^\varphi} (N_b^\varphi)_{,l} g_{k(b)} \quad (19)$$

where $d_{k(a)}$ is the displacement vector at node a, $\phi_{l(b)}$ is the rotation vector at node b, $c_{k(a)}$ is the displacement weighting function vector at node a, $g_{k(b)}$ is the rotation weighting function vector at node b, n_{en}^u is the number of element nodes associated with interpolating the continuum macrodisplacement vector, and n_{en}^φ is the number of element nodes associated with interpolating the continuum microrotation vector. It is assumed that the shape functions and integrals are expressed in natural coordinates for an isoparametric formulation, but such details are omitted and can be found in the textbook by Hughes [6]. Substituting these approximations into the Galerkin form, accounting for essential boundary conditions, and recognizing that the nodal weighting function values are arbitrary (except where essential boundary conditions are applied, and nodal weighting function values are zero), we arrive at a coupled matrix form of the linear and angular momentum balance equations

$$\boldsymbol{M}^u \ddot{\boldsymbol{d}} + \boldsymbol{F}^{INT,u}(\boldsymbol{d},\boldsymbol{\phi}) = \boldsymbol{F}_b + \boldsymbol{F}_t \quad (20)$$
$$\boldsymbol{M}^\varphi \ddot{\boldsymbol{\phi}} + \boldsymbol{F}^{INT,\varphi}(\boldsymbol{d},\boldsymbol{\phi}) = \boldsymbol{F}_\ell + \boldsymbol{F}_r \quad (21)$$

where matrices and vectors are assembled from their element contributions using the traditional finite element assembly operator [6]

$$\boldsymbol{M}^{u} = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}^e} \rho(\boldsymbol{N}_e^u)^T \boldsymbol{N}_e^u dv \tag{22}$$

$$\boldsymbol{M}^{\varphi} = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}^e} \rho(\boldsymbol{N}_e^\varphi)^T \boldsymbol{j}^T \boldsymbol{N}_e^\varphi dv \tag{23}$$

$$\boldsymbol{F}^{INT,u}(\boldsymbol{d},\boldsymbol{\phi}) = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}^e} (\boldsymbol{B}_e^u)^T \boldsymbol{\sigma}(\boldsymbol{d}^e,\boldsymbol{\phi}^e) dv \tag{24}$$

$$\begin{aligned}\boldsymbol{F}^{INT,\varphi}(\boldsymbol{d},\boldsymbol{\phi}) = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \Bigg(& \int_{\mathcal{B}^e} (\boldsymbol{B}_e^\varphi)^T \boldsymbol{m}(\boldsymbol{d}^e,\boldsymbol{\phi}^e) dv \\ & - \int_{\mathcal{B}^e} (\boldsymbol{N}_e^\varphi)^T \boldsymbol{\sigma}^\epsilon(\boldsymbol{d}^e,\boldsymbol{\phi}^e) dv \Bigg)\end{aligned} \tag{25}$$

$$\boldsymbol{F}_b = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}^e} \rho(\boldsymbol{N}_e^u)^T \boldsymbol{b} dv \tag{26}$$

$$\boldsymbol{F}_\ell = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}^e} \rho(\boldsymbol{N}_e^\varphi)^T \boldsymbol{\ell} dv \tag{27}$$

$$\boldsymbol{F}_t = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\Gamma_t^e} (\boldsymbol{N}_e^u)^T \boldsymbol{t} da \tag{28}$$

$$\boldsymbol{F}_r = \mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}} \int_{\Gamma_r^e} (\boldsymbol{N}_e^\varphi)^T \boldsymbol{r} da \tag{29}$$

where $\mathop{\mathbf{A}}_{e=1}^{n_{\mathrm{el}}}$ is the element assembly operator, n_{el} is the number of elements, $\boldsymbol{N}_e^u$, $\boldsymbol{N}_e^\varphi$, $\boldsymbol{j}$, $\boldsymbol{B}_e^u$, $\boldsymbol{\sigma}$, $\boldsymbol{d}^e$, $\boldsymbol{\phi}^e$, $\boldsymbol{B}_e^\varphi$, $\boldsymbol{m}$, $\boldsymbol{\sigma}^\epsilon$, $\boldsymbol{b}$, $\boldsymbol{\ell}$, $\boldsymbol{t}$, and $\boldsymbol{r}$ are the element matrix and vector forms of N_a^u, N_b^φ, j_{lk}, $(N_a^u)_{,l}$, σ_{lk}, $d_{k(a)}$, $\phi_{l(b)}$, $(N_b^\varphi)_{,l}$, m_{lk}, $\epsilon_{kmn}\sigma_{mn}$, b_k, ℓ_k, t_k, and r_k, respectively [6].

Introducing a generalized nodal degree of freedom vector $\boldsymbol{D}$, the coupled micropolar linear and angular momentum balance equations are written as

$$\boldsymbol{M}^D \ddot{\boldsymbol{D}} + \boldsymbol{F}^{INT,D}(\boldsymbol{D}) = \boldsymbol{F}^{EXT,D} \tag{30}$$

$$\begin{aligned}\boldsymbol{M}^D &= \begin{bmatrix} \boldsymbol{M}^u & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M}^\varphi \end{bmatrix} \quad \boldsymbol{D} = \begin{bmatrix} \boldsymbol{d} \\ \boldsymbol{\phi} \end{bmatrix} \\ \boldsymbol{F}^{INT,D} &= \begin{bmatrix} \boldsymbol{F}^{INT,u} \\ \boldsymbol{F}^{INT,\varphi} \end{bmatrix} \quad \boldsymbol{F}^{EXT,D} = \begin{bmatrix} \boldsymbol{F}_b + \boldsymbol{F}_t \\ \boldsymbol{F}_\ell + \boldsymbol{F}_r \end{bmatrix}\end{aligned} \tag{31}$$

With regard to putting the continuum micropolar mechanics and finite element implementation into a form amenable to energy partitioning in the coupled particle-continuum overlap region, we consider an energy formulation of the balance equations using Lagrange's equation of motion. It may be stated as

$$\frac{d}{dt}\left(\frac{\partial T^D}{\partial \dot{\boldsymbol{D}}}\right) - \frac{\partial T^D}{\partial \boldsymbol{D}} + \frac{\partial F^D}{\partial \dot{\boldsymbol{D}}} + \frac{\partial U^D}{\partial \boldsymbol{D}} = \boldsymbol{F}^{EXT,D} \tag{32}$$

where T^D is the kinetic energy, F^D the dissipation function, and U^D the potential energy, such that

$$T^D = \frac{1}{2}\dot{\boldsymbol{D}}\boldsymbol{M}^D\dot{\boldsymbol{D}} \tag{33}$$

$$F^D = 0 \tag{34}$$

$$U^D(\boldsymbol{D}) = \int_{\boldsymbol{0}}^{\boldsymbol{D}} \boldsymbol{F}^{INT,D}(\boldsymbol{S}) d\boldsymbol{S} \tag{35}$$

Carrying out the derivation in Eq.(32) leads to Eq.(30), assuming constant inertia $\boldsymbol{M}^D$.

COUPLING METHOD

An aspect of the computational multiscale modeling approach is to couple regions of material represented by particles, Discrete Element (DE), to regions of material represented by continuum, Finite Element (FE). Another aspect is to bridge the particle mechanics to a continuum representation using micromorphic plasticity [7], whereas the linear micropolar elastic continuum is a simple approximation of glued, stiff, elastic particles. The coupling implementation will allow arbitrarily overlapping particle and continuum regions in a single hand-shaking or overlap region such that fictitious forces and wave reflections are minimized in the overlap region. In theory, for nearly homogeneous deformations, if the particle and continuum regions share the same region (i.e., are completely overlapped), the results should be the same as if the overlap region is a subset of the overall problem domain (cf. Fig.1). This will serve as a future benchmark problem for the numerical implementation. The coupling implementation proposed in this research follows the "bridging scale decomposition" proposed by Wagner and Liu [1] and modifications thereof by Klein and Zimmerman [2] (the terminology "bridging" of scales in [1] is what we refer to as coupling of regions in this work). The potential energy partitioning method described in [2] will be a point of departure for our particle-continuum coupling implementation and extension to include dynamics (kinetic energy).

Kinematics

Here, a summary of the kinematics of the coupled regions is given, following the illustration shown in Fig.1. It is assumed that the finite element mesh covers the domain of the problem in which the material is behaving more solid-like, whereas in regions of large relative particle motion (fluid-like), a particle mechanics representation is used (DE). But for generality, we will formulate the kinematics assuming the particle and continuum domains could completely overlap, or one contained within the other. Following some of the same notation presented in [1, 2], we define a generalized degree of freedom (dof) vector $\breve{\boldsymbol{Q}}$ for particle displacements and rotations in the system as

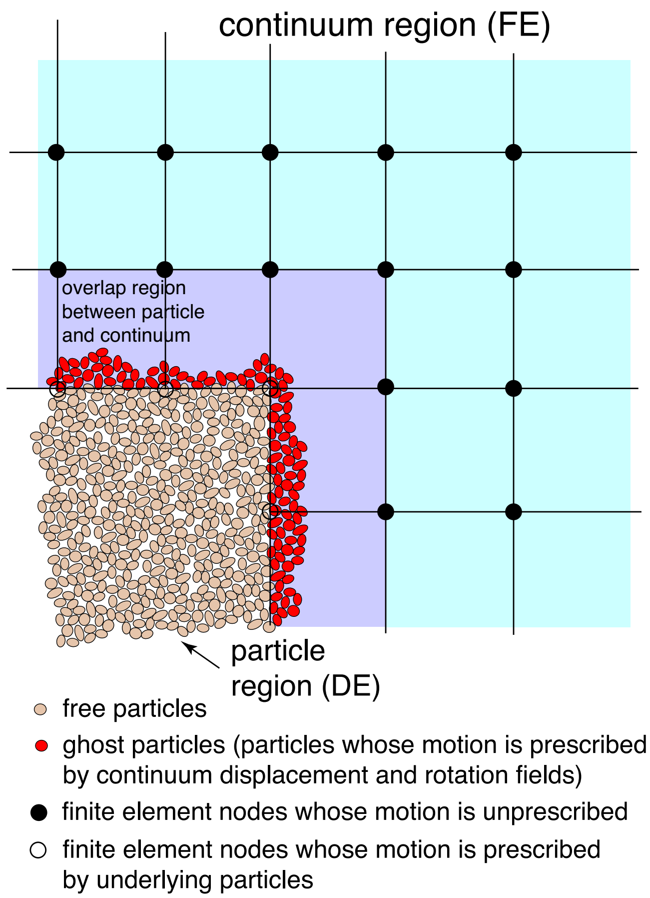

Figure 1. Two-dimensional illustration of the coupling between particle and continuum regions. The purple background denotes the overlap region, light blue the continuum region, and white background (with brown particles) the particle region.

$$\breve{\boldsymbol{Q}} = [\boldsymbol{q}_\alpha, \boldsymbol{q}_\beta, \ldots, \boldsymbol{q}_\gamma, \boldsymbol{\theta}_\alpha, \boldsymbol{\theta}_\beta, \ldots, \boldsymbol{\theta}_\gamma]^T, \ \alpha, \beta, \ldots, \gamma \in \breve{\mathcal{A}} \tag{36}$$

where $\boldsymbol{q}_\alpha$ is the displacement vector of particle α, $\boldsymbol{\theta}_\alpha$ its rotation vector, and $\breve{\mathcal{A}}$ is the set of all particles. Likewise, the finite element nodal displacements and rotations are written as

$$\begin{gathered}\breve{\boldsymbol{D}} = [\boldsymbol{d}_a, \boldsymbol{d}_b, \ldots, \boldsymbol{d}_c, \boldsymbol{\phi}_d, \boldsymbol{\phi}_e, \ldots, \boldsymbol{\phi}_f]^T \\ a, b, \ldots, c \in \breve{\mathcal{N}} \ , \quad d, e, \ldots, f \in \breve{\mathcal{M}}\end{gathered} \tag{37}$$

where $\boldsymbol{d}_a$ is the displacement vector of node a, $\boldsymbol{\phi}_d$ is the rotation vector of node d, $\breve{\mathcal{N}}$ is the set of all nodes, and $\breve{\mathcal{M}}$ is the set of finite element nodes with rotational degrees of freedom, where $\breve{\mathcal{M}} \subset \breve{\mathcal{N}}$. In order to satisfy the boundary conditions for both regions, the motion of the particles in the overlap region (referred to as "ghost particles," cf. Fig.1) is prescribed by the continuum displacement and rotation fields, and written as

$$\widehat{\boldsymbol{Q}} = [\boldsymbol{q}_\alpha, \boldsymbol{q}_\beta, \ldots, \boldsymbol{q}_\gamma, \boldsymbol{\theta}_\alpha, \boldsymbol{\theta}_\beta, \ldots, \boldsymbol{\theta}_\gamma]^T, \ \alpha, \beta, \ldots, \gamma \in \widehat{\mathcal{A}} \tag{38}$$

while the unprescribed (or free) particle displacements and rotations are

$$\boldsymbol{Q} = [\boldsymbol{q}_\delta, \boldsymbol{q}_\epsilon, \ldots, \boldsymbol{q}_\eta, \boldsymbol{\theta}_\delta, \boldsymbol{\theta}_\epsilon, \ldots, \boldsymbol{\theta}_\eta]^T \ , \quad \delta, \epsilon, \ldots, \eta \in \mathcal{A} \tag{39}$$

where $\widehat{\mathcal{A}} \cup \mathcal{A} = \breve{\mathcal{A}}$ and $\widehat{\mathcal{A}} \cap \mathcal{A} = \emptyset$. Likewise, the displacements and rotations of nodes overlaying the particle region are prescribed by the particle motion and written as

$$\begin{gathered}\widehat{\boldsymbol{D}} = [\boldsymbol{d}_a, \boldsymbol{d}_b, \ldots, \boldsymbol{d}_c, \boldsymbol{\phi}_d, \boldsymbol{\phi}_e, \ldots, \boldsymbol{\phi}_f]^T \\ a, b, \ldots, c \in \widehat{\mathcal{N}} \ , \quad d, e, \ldots, f \in \widehat{\mathcal{M}}\end{gathered} \tag{40}$$

while the unprescribed (or free) nodal displacements and rotations are

$$\begin{gathered}\boldsymbol{D} = [\boldsymbol{d}_m, \boldsymbol{d}_n, \ldots, \boldsymbol{d}_s, \boldsymbol{\phi}_t, \boldsymbol{\phi}_u, \ldots, \boldsymbol{\phi}_v]^T \\ m, n, \ldots, s \in \mathcal{N} \ , \quad t, u, \ldots, v \in \mathcal{M}\end{gathered} \tag{41}$$

where $\widehat{\mathcal{N}} \cup \mathcal{N} = \breve{\mathcal{N}}$, $\widehat{\mathcal{N}} \cap \mathcal{N} = \emptyset$, $\widehat{\mathcal{M}} \cup \mathcal{M} = \breve{\mathcal{M}}$, and $\widehat{\mathcal{M}} \cap \mathcal{M} = \emptyset$.

In general, the displacement vector of a particle α can be represented by the finite element interpolation of the continuum macrodisplacement field $\boldsymbol{u}^h$ evaluated at the particle centroid in the reference configuration $\boldsymbol{X}_\alpha$, such that

$$\boldsymbol{u}^h(\boldsymbol{X}_\alpha, t) = \sum_{a \in \breve{\mathcal{N}}} N_a^u(\boldsymbol{X}_\alpha)\boldsymbol{d}_a(t) \quad \alpha \in \breve{\mathcal{A}} \tag{42}$$

where N_a^u are the shape functions associated with the continuum displacement field $\boldsymbol{u}^h$. Recall that N_a^u have compact support and thus are only evaluated for particles that lie within an element containing node a in its domain. For example, we can write the prescribed displacement of ghost particle α as

$$\boldsymbol{q}_\alpha(t) = \boldsymbol{u}^h(\boldsymbol{X}_\alpha, t) = \sum_{a \in \breve{\mathcal{N}}} N_a^u(\boldsymbol{X}_\alpha)\boldsymbol{d}_a(t) \quad \alpha \in \widehat{\mathcal{A}} \tag{43}$$

Likewise, particle rotation vectors can be represented by the finite element interpolation of the continuum microrotation field $\boldsymbol{\varphi}^h$ evaluated at the particle centroid in the reference configuration $\boldsymbol{X}_\alpha$, such that

$$\boldsymbol{\varphi}^h(\boldsymbol{X}_\alpha, t) = \sum_{b \in \breve{\mathcal{M}}} N_b^\varphi(\boldsymbol{X}_\alpha)\boldsymbol{\phi}_b(t) \quad \alpha \in \breve{\mathcal{A}} \tag{44}$$

where N_b^φ are the shape functions associated with the microrotation field $\boldsymbol{\varphi}^h$. For example, we can write the prescribed rotation of ghost particle α as

$$\boldsymbol{\theta}_\alpha(t) = \boldsymbol{\varphi}^h(\boldsymbol{X}_\alpha, t) = \sum_{b \in \breve{\mathcal{M}}} N_b^\varphi(\boldsymbol{X}_\alpha)\boldsymbol{\phi}_b \quad \alpha \in \widehat{\mathcal{A}} \tag{45}$$

For all ghost particles, the interpolations can be written as

$$\widehat{\boldsymbol{Q}} = \boldsymbol{N}_{\widehat{Q}D} \cdot \boldsymbol{D} + \boldsymbol{N}_{\widehat{Q}\widehat{D}} \cdot \widehat{\boldsymbol{D}} \tag{46}$$

where $\boldsymbol{N}_{\widehat{Q}D}$ and $\boldsymbol{N}_{\widehat{Q}\widehat{D}}$ are shape function matrices containing individual nodal shape functions N_a^u and N_b^φ, but for now these matrices will be left general to increase our flexibility in choosing interpolation functions (such as those used in meshfree methods). Overall, the particle displacements and rotations may be written as

$$\begin{bmatrix} \boldsymbol{Q} \\ \widehat{\boldsymbol{Q}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{N}_{QD} & \boldsymbol{N}_{Q\widehat{D}} \\ \boldsymbol{N}_{\widehat{Q}D} & \boldsymbol{N}_{\widehat{Q}\widehat{D}} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{D} \\ \widehat{\boldsymbol{D}} \end{bmatrix} + \begin{bmatrix} \boldsymbol{Q}' \\ \boldsymbol{0} \end{bmatrix} \tag{47}$$

where $\boldsymbol{Q}'$ is introduced as the error in the interpolation of the free particle displacements and rotations $\boldsymbol{Q}$, whose function space is not rich enough to represent the true free particle motion. The shape function matrices $\boldsymbol{N}$ are in general not square because the number of free particles are not the same as free nodes and prescribed nodes, and number of ghost particles not the same as prescribed and free nodes. Thus, a scalar measure of error in particle displacements and rotations is defined as

$$e = \boldsymbol{Q}' \cdot \boldsymbol{Q}' \tag{48}$$

which may be minimized to solve for prescribed particle and nodal displacements and rotations $\widehat{\boldsymbol{Q}}$ and $\widehat{\boldsymbol{D}}$ in terms of their free counterparts $\boldsymbol{Q}$ and $\boldsymbol{D}$. Following the procedure in [2], upon minimizing e in Eq.(48), we can solve for the prescribed particle and nodal degrees of freedom as

$$\widehat{\boldsymbol{Q}} = \boldsymbol{B}_{\widehat{Q}Q}\boldsymbol{Q} + \boldsymbol{B}_{\widehat{Q}D}\boldsymbol{D} \tag{49}$$

$$\widehat{\boldsymbol{D}} = \boldsymbol{B}_{\widehat{D}Q}\boldsymbol{Q} + \boldsymbol{B}_{\widehat{D}D}\boldsymbol{D} \tag{50}$$

where

$$\boldsymbol{B}_{\widehat{Q}Q} = \boldsymbol{N}_{\widehat{Q}\widehat{D}}\boldsymbol{N}^{-1}_{Q\widehat{D}} \tag{51}$$

$$\boldsymbol{B}_{\widehat{Q}D} = \boldsymbol{N}_{\widehat{Q}D} - \boldsymbol{B}_{\widehat{Q}Q}\boldsymbol{N}_{QD} \tag{52}$$

$$\boldsymbol{B}_{\widehat{D}Q} = \boldsymbol{N}^{-1}_{Q\widehat{D}} \tag{53}$$

$$\boldsymbol{B}_{\widehat{D}D} = -\boldsymbol{N}^{-1}_{Q\widehat{D}}\boldsymbol{N}_{QD} \tag{54}$$

Kinetic and Potential Energy Partitioning and Coupling

We assume the total kinetic and potential energy of the coupled particle-continuum system may be written as the sum of the energies

$$T(\dot{\boldsymbol{Q}}, \dot{\boldsymbol{D}}) = T^Q(\dot{\boldsymbol{Q}}, \dot{\widehat{\boldsymbol{Q}}}(\dot{\boldsymbol{Q}}, \dot{\boldsymbol{D}})) + T^D(\dot{\boldsymbol{D}}, \dot{\widehat{\boldsymbol{D}}}(\dot{\boldsymbol{Q}}, \dot{\boldsymbol{D}})) \tag{55}$$

$$U(\boldsymbol{Q}, \boldsymbol{D}) = U^Q(\boldsymbol{Q}, \widehat{\boldsymbol{Q}}(\boldsymbol{Q}, \boldsymbol{D})) + U^D(\boldsymbol{D}, \widehat{\boldsymbol{D}}(\boldsymbol{Q}, \boldsymbol{D})) \tag{56}$$

where we have indicated the functional dependence of the prescribed particle motion and nodal dofs solely upon the free particle motion and nodal dofs $\boldsymbol{Q}$ and $\boldsymbol{D}$, respectively. Note that in taking the time derivatives $\dot{\widehat{\boldsymbol{Q}}}$ and $\dot{\widehat{\boldsymbol{D}}}$ we assume either the kinematics are linear (small strain), or that the shape functions are evaluated in the reference configuration. These are details for the actual numerical implementation, but we will pursue a finite deformation finite element implementation. Lagrange's equations may then be stated as

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\boldsymbol{Q}}}\right) - \frac{\partial T}{\partial \boldsymbol{Q}} + \frac{\partial F}{\partial \dot{\boldsymbol{Q}}} + \frac{\partial U}{\partial \boldsymbol{Q}} &= \boldsymbol{F}^{EXT,Q} \\ \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\boldsymbol{D}}}\right) - \frac{\partial T}{\partial \boldsymbol{D}} + \frac{\partial F}{\partial \dot{\boldsymbol{D}}} + \frac{\partial U}{\partial \boldsymbol{D}} &= \boldsymbol{F}^{EXT,D} \end{aligned} \tag{57}$$

which lead to a coupled system of governing equations (linear and angular momentum) for the coupled particle-continuum mechanics in the overlap region. The derivatives are

$$\frac{\partial T}{\partial \dot{\boldsymbol{Q}}} = \frac{\partial T^Q}{\partial \dot{\boldsymbol{Q}}} + \frac{\partial T^Q}{\partial \dot{\widehat{\boldsymbol{Q}}}}\boldsymbol{B}_{\widehat{Q}Q} + \frac{\partial T^D}{\partial \dot{\widehat{\boldsymbol{D}}}}\boldsymbol{B}_{\widehat{D}Q} \tag{58}$$

$$\frac{\partial T}{\partial \boldsymbol{Q}} = \boldsymbol{0} \tag{59}$$

$$\frac{\partial F}{\partial \dot{\boldsymbol{Q}}} = \frac{\partial F^Q}{\partial \dot{\boldsymbol{Q}}} = a\left(\frac{\partial T^Q}{\partial \dot{\boldsymbol{Q}}} + \frac{\partial T^Q}{\partial \dot{\widehat{\boldsymbol{Q}}}}\boldsymbol{B}_{\widehat{Q}Q}\right) \tag{60}$$

$$\frac{\partial U}{\partial \boldsymbol{Q}} = \frac{\partial U^Q}{\partial \boldsymbol{Q}} + \frac{\partial U^Q}{\partial \widehat{\boldsymbol{Q}}}\boldsymbol{B}_{\widehat{Q}Q} + \frac{\partial U^D}{\partial \widehat{\boldsymbol{D}}}\boldsymbol{B}_{\widehat{D}Q} \tag{61}$$

$$\frac{\partial T}{\partial \dot{\boldsymbol{D}}} = \frac{\partial T^D}{\partial \dot{\boldsymbol{D}}} + \frac{\partial T^D}{\partial \dot{\widehat{\boldsymbol{D}}}}\boldsymbol{B}_{\widehat{D}D} + \frac{\partial T^Q}{\partial \dot{\widehat{\boldsymbol{Q}}}}\boldsymbol{B}_{\widehat{Q}D} \tag{62}$$

$$\frac{\partial T}{\partial \boldsymbol{D}} = \boldsymbol{0} \tag{63}$$

$$\frac{\partial F}{\partial \dot{\boldsymbol{D}}} = \boldsymbol{0} \tag{64}$$

$$\frac{\partial U}{\partial \boldsymbol{D}} = \frac{\partial U^D}{\partial \boldsymbol{D}} + \frac{\partial U^D}{\partial \widehat{\boldsymbol{D}}}\boldsymbol{B}_{\widehat{D}D} + \frac{\partial U^Q}{\partial \widehat{\boldsymbol{Q}}}\boldsymbol{B}_{\widehat{Q}D} \tag{65}$$

If the potential energy U is nonlinear with regard to particle frictional sliding and micropolar (or micromorphic) plasticity, then Eqs.(57) may be integrated in time and linearized for solution by the Newton-Raphson method, as we will do.

SUMMARY

The paper presented the formulation for coupling particle and micropolar elastic continuum mechanics regions of a particulate material, following the lattice-based approaches described in [1,2], but extending to rotational dofs and kinetic energy. For the case of large particle motion and frictional sliding, a finite deformation micromorphic plasticity model would need to be coupled to the particle mechanics within the overlap region. Such a model for particulate materials is being formulated and will be presented in a later paper [7]. We believe a micropolar plasticity model would be insufficient, missing the microstretch and microshear that clusters of particles could demonstrate, in addition to microrotations. The eventual multiscale computational approach is meant to account for the particle mechanics (actual particle size) in regions of large relative particle motion or flow, and for the approximate continuum behavior in adjacent and far-field regions.

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