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MULTISCALE ANALYSES OF GRANULAR MEDIA AT FINITE STRAINS BASED ON MICRO–MACRO TRANSITIONS WITH DIFFERENT BOUNDARY CONSTRAINTS

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Summary Considered is a homogenized macro–continuum with locally attached microstructures of discrete character. For example, these microstructures may represent granular assemblies of particles used in analyses in soil mechanics or aggregates of atoms for analyses in nanoscale mechanics of metals. Specific micro–macro transitions are derived by a consistent transfer of the discrete micro–variables to macroscopic field variables on a continuous (smeared) macrostructure. On the microscopic side, the classical boundary conditions of homogenization theory of continuous structures are consistently transferred to their discrete counterparts including the effect of particle rotations. It is shown that those for linear displacements and uniform tractions on the surface yield upper and lower bound characteristics, respectively, for the periodic boundary constraints with regard to the stiffness of the aggregate. Therein, special attention is paid to the definition of the periodic unit cell of granular particles which leads to specific constraints for both displacements and rotations of the granules on the well–defined boundary frame of the microstructure. On the macroscopic side, the homogeneous problem is solved by a finite element method where the material model is implemented by means of directly evaluated micro–macro transitions based on the above mentioned discrete microstructures for the case of periodic boundary constraints. Thus, the two–scale simulations are linked by solving coupled boundary–value problems on both the micro– and macroscales. Finally, some representative numerical examples are investigated and discussed which underline and clarify the proposed method.

Introduction

Within the classical setting of large–strain continuum mechanics, phenomenological macroscopic material models are developed where the material parameters are fitted according to experimental observations. In recent years, attention has been shifted to multiscale analyses of materials where the real microscopic structures of such materials are accounted for. Many materials show discrete microstructures such as granular media like soils and sand or even metals with a discrete, particulate–like atomistic structure on the nanoscale. So far, in the modeling of discrete granular structures, attention has mostly been paid to the simulation of the evolution of microstructures, not its embedding into large–scale macroscopic simulations. With the advent of powerful computers, coupled micro–macro analyses of those problems are only the next logical step. Figure 1 shows a homogenized macro–continuum where a microstructure is attached locally

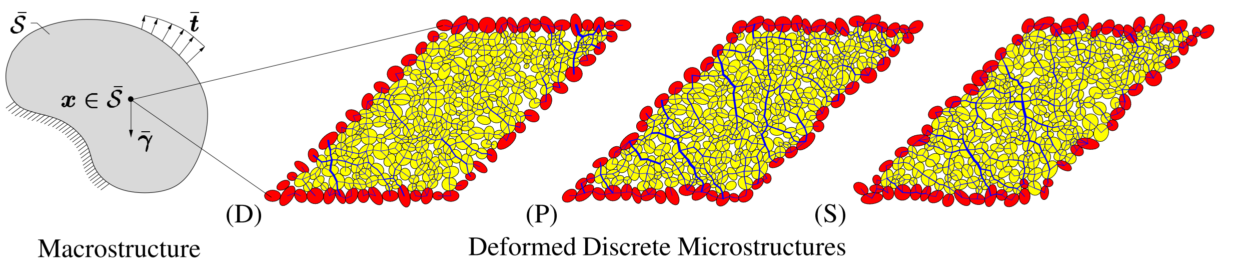

Figure 1. Deformed continuous macrostructure with a granular microstructure locally attached at a point $\bar{x} \in \bar{\mathcal{S}}$ under (D) linear deformations, (P) periodic displacements and (S) uniform traction constraints on the surface of the representative volume element.

at a point $\bar{\boldsymbol{X}} \in \mathcal{S}$ of the macrostructure and deformed in a compression–shear mode. A micro–macro transition of such a discrete aggregate is concerned with the definition of homogenized overall properties such as strains, stresses and powers. A central difference to other works on granular microstructures is a distinct definition of the aggregate volume and its boundary conditions which govern the representation of the macro–stresses. A well–defined periodic cell allows a consistent transfer of overall definitions for continuous microstructures of heterogeneous materials to discrete particle microstructures. Recall from classical homogenization theory that periodicity conditions reflect exact results with regard to the aggregate stiffness for periodic structures, while linear deformation and uniform traction constraints yield upper and lower bound characteristics, respectively. It will be shown that these statements also hold true for granular materials. Consequently, the proposed periodicity conditions are considered to be an optimal choice for particle aggregate and will thus be used for the proposed *two–scale micro–macro simulations* where we link boundary–value problems on both the micro– and macroscales.

Micromechanical modeling

For analyses of granular materials, the discrete element method has become a popular tool. Microscopic constitutive equations for the discrete particle interactions are introduced which govern the macroscopic response by computational exploitation of micro–macro averaging theorems. In each incremental step the current branch meshes are computed and the equation of motion is solved for all particles until quasistatic equilibrium states are reached. An optimized technique that accelerates the dynamic relaxation procedure is introduced. The Cauchy macro–stresses are the volume average of the Cauchy micro–stresses and appear in the form $\bar{\boldsymbol{\sigma}} = \frac{1}{2|v|}\sum_q(\boldsymbol{f}_q \otimes \boldsymbol{x}_q + \boldsymbol{x}_q \otimes \boldsymbol{f}_q)$ where we sum over only the M

particles on the defined boundary frame the actual particle positions $\boldsymbol{x}_q$ and externally applied support forces $\boldsymbol{f}_q$. Note that due to our distinct definition of the boundary frame only the particle–centroid forces enter the stress formulation. For periodic boundary conditions, all couples drop out due to the antiperiodicity condition and thus do not influence the stress calculation. The three classical boundary constraints for continuous structures, see [2], are consistently transferred to their discrete counterparts. In order to implement these into a deformation–driven scenario, for the particle–centroid interaction forces of all particles in the aggregate we assume potentials which need to be minimized. Therein, special assumptions are made for the particle rotations in the cases of linear displacement and uniform traction constraints. The boundary constraints are then incorporated by a penalty method in the form of quadratic terms such that for the three boundary constraints we end up with the fictitious potentials

$$\begin{array}{lll} \text{(D)} \quad \Pi_p^D(\boldsymbol{x}_q, \boldsymbol{Q}_q) & = & \Pi(\boldsymbol{x}_q) + \frac{\epsilon_f}{2}\sum_{q=1}^{M} ||\boldsymbol{x}_q - \bar{\boldsymbol{F}}\boldsymbol{X}_q||^2 + \frac{\epsilon_c}{4}\sum_{q=1}^{M} ||\boldsymbol{Q}_q - \boldsymbol{1}||^2 \\ \text{(P)} \quad \Pi_p^P(\boldsymbol{x}_q, \boldsymbol{Q}_q) & = & \Pi(\boldsymbol{x}_q) + \frac{\epsilon_f}{2}\sum_{q=1}^{M^+} ||\, [\![\boldsymbol{x}_q]\!] - \bar{\boldsymbol{F}}\, [\![\boldsymbol{X}_q]\!]\, ||^2 + \frac{\epsilon_c}{4}\sum_{q=1}^{M^+} ||\, [\![\boldsymbol{Q}_q]\!]\, ||^2 \\ \text{(S)} \quad \Pi_p^S(\boldsymbol{x}_q) & = & \Pi(\boldsymbol{x}_q) + \frac{\epsilon_f}{2}||\sum_{q=1}^{M}(\boldsymbol{x}_q \otimes \boldsymbol{A}_q) - |\mathcal{V}|\bar{\boldsymbol{F}}||^2 \end{array} \quad (1)$$

Derivations of these particle interaction force–potentials with respect to the actual positions $\boldsymbol{x}_q$ and rotations ϑ_q then give the support forces $\boldsymbol{f}_q$ and couples m_q needed to attain the boundary constraint considered:

$$\begin{array}{llllll} \text{(D)} \quad \boldsymbol{f}_q & = & \epsilon_f(\boldsymbol{x}_q - \bar{\boldsymbol{F}}\boldsymbol{X}_q)\,, & m_q & = & \epsilon_c(\vartheta_q - \Theta_q) \\ \text{(P)} \quad \boldsymbol{f}_q^+ & = & \epsilon_f([\![\boldsymbol{x}_q]\!] - \bar{\boldsymbol{F}}[\![\boldsymbol{X}_q]\!]) = -\boldsymbol{f}_q\,, & m_q^+ & = & \epsilon_c[\![\vartheta_q]\!] = -m_q^- \\ \text{(S)} \quad \boldsymbol{f}_q & = & \epsilon_f[\sum_p(\boldsymbol{A}_p \cdot \boldsymbol{A}_q)\boldsymbol{x}_p - |\mathcal{V}|\bar{\boldsymbol{F}} \cdot \boldsymbol{A}_q]\,, & m_q & = & 0 \end{array} \quad (2)$$

where ϵ_f and ϵ_c are penalty factors, $\boldsymbol{Q}$ is a proper orthogonal rotation tensor and $\boldsymbol{A}_q$ an outward area normal vector on the undeformed surface of the microstructure. ϑ_q and Θ_q are the actual and referential rotations of a particle q. Figure 2 shows homogenized normal and shear stresses versus a macroscopic simple shear deformation mode for a typical microstructure made of 256 elliptical particles as shown in Figure 1. The bound character of the linear displacement and uniform traction constraints with respect to the periodic conditions is clearly obvious.

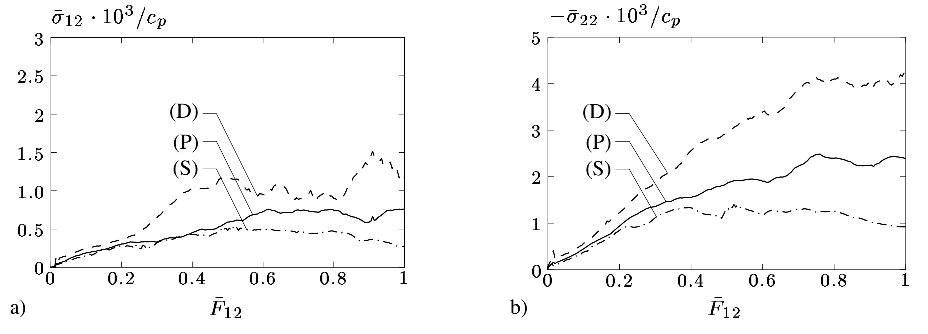

Figure 2. Homogenized a) shear stresses $\bar{\sigma}_{12}$ and b) compressive stresses $-\bar{\sigma}_{22}$ versus macroscopic shear deformation $\bar{F}_{12}$ for the three types of boundary conditions (D) linear displacements, (P) periodic deformations and (S) uniform tractions on the surface. The simulation was carried out with a granular plane microstructure of 256 elliptically–shaped particles.

Macroscopic Finite Element Modeling

The point of departure for the finite element method is the strong form of quasistatic equilibrium. A Galerkin procedure and some algebraic manipulations yield the weak counterpart, further discretization finally the well–known form $\int_{\bar{\mathcal{B}}} \boldsymbol{B}^T \cdot \bar{\boldsymbol{P}}(\boldsymbol{d})\, dV = \int_{\bar{\mathcal{B}}} \boldsymbol{N}^T \cdot \bar{\gamma}\, dV + \int_{\partial\bar{\mathcal{B}}} \boldsymbol{N}^T \cdot \bar{\boldsymbol{t}}\, dA$. The left hand side of the equation are the internal forces that depend on the actual nodal displacements $\boldsymbol{d}$ and thus on the deformed particulate microstructure. The first Piola–Kirchhoff stresses $\bar{\boldsymbol{P}}$ are determined by direct evaluation of micro–macro transitions on the microscale. This is done at each sampling point of the finite element by passing the increment of the actual deformation gradient in each step onto the microstructure, where then the microscopic simulation is carried out, the macroscopic stress determined and passed back to the macroscale. This step marks the link between the simulations on both scales. We apply an explicit solution strategy in context with an accelerated dynamic relaxation procedure. After each load step the system is iteratively solved until the quasistatic equilibrium configuration is reached.

References

[1] Miehe C., Dettmar, J.: A framework for micro–macro transitions in periodic particle aggregates of granular materials, *Computer Methods in Applied Mechanics and Engineering*, **193**: 225-256, 2004.

[2] Miehe C.: Computational micro–to–macro transitions for dicretized micro–structures of heterogeneous materials at finite strains based on the minimization of averaged incremental energy, *Computer Methods in Applied Mechanics and Engineering*, **192**:559–591, 2003.

[3] Miehe C., Dettmar, J.: A new class of boundary conditions for micro–macro transitions in particle aggregates of granular materials, *International Journal of Solids and Structures*, submitted.