MULTISCALE MODELING OF GRANULAR MATERIALS USING MESOSCALE DEM AND MACHINE LEARNING APPROACHES

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Abstract: We establish the necessary framework for inputting any kind of mesostructure into multiscale models for granular materials. Keeping intact the general statistical homogenization scheme, we propose a strategy to compute the mechanical response of the mesostructures directly with discrete element simulations of a few grains or thanks to surrogate models relying on artificial neuron networks (ANN). By applying machine learning techniques at the mesoscale (instead of the Representative Elementary Volume scale), it is indeed possible to generate the necessary learning database from discrete element simulations at a relatively cheap computational cost. We apply the meso-DEM and meso-ANN strategies to the H-model (one particular micromechanical model), and we show that they can replicate the original analytical expression of the model on biaxial tests. This work paves the way for using more complex mesostructures to account for instance for gap-graded materials.

1. Introduction

When it comes to deriving the constitutive behavior of a heterogeneous material from a detailed description of its microstructure, two homogenization strategies can be employed, namely spatial homogenization or statistical homogenization. On the one hand, spatial homogenization is based on the concept of the representative elementary volume (REV), and the constitutive relationships are obtained by computing the volume averages of local stresses and strains. On the other hand, statistical homogenization is based on the description of the microstructure as a collection of independent features with simple mechanical behavior. The macroscopic behavior is then obtained as a weighted average of the responses of all the simple mechanical systems. Taylor opened the way for the development of such constitutive models with the so-called multislip (or multiplane) theory [1]. This theory was adapted later to geomaterials and gave rise to microplane models (see for instance [2, 3]) with a fractured continuum media in mind. But for granular media, the statistical description of the microstrucutre only by contact planes proved to be too poor, as local arrangements of a few grains form mesostructures responsible for a myriad of emerging properties [4, 5]. Therefore, the current challenge faced by most multiscale models based on statistical homogenization is to incorporate sufficient relevant microstructural features into the simplified mesostructures for complex properties to emerge during the upscaling process.

For granular materials, one particular example of multiscale models that embed explicitely a mesostructure is the H-model [6, 7, 8]. This model relies on elementary mesostructures that consist in hexagonal patterns of six circular grains in 2D and bi-hexagonal patterns of ten spherical grains in 3D (the "H-cell"). Because of the imposed H-cell symmetry, the mechanical response of the model is analytically derivable. However, the model suffers from several known limitations, which will require the use of enriched mesostructures probably too complex for an analytical treatment. In particular, the model cannot account for the behavior of widely graded materials and the possible consequences of internal erosion since the H-cell is formed of grains of equal radii. In the present work, we propose to waive the analytical resolution of the mesoscale behavior of the H-model while keeping intact the homogenization scheme of the model recalled in Figure 1. Instead, we propose meso-DEM (discrete element method) and meso-ANN (artificial neuron network) strategies to solve the H-cell behavior.

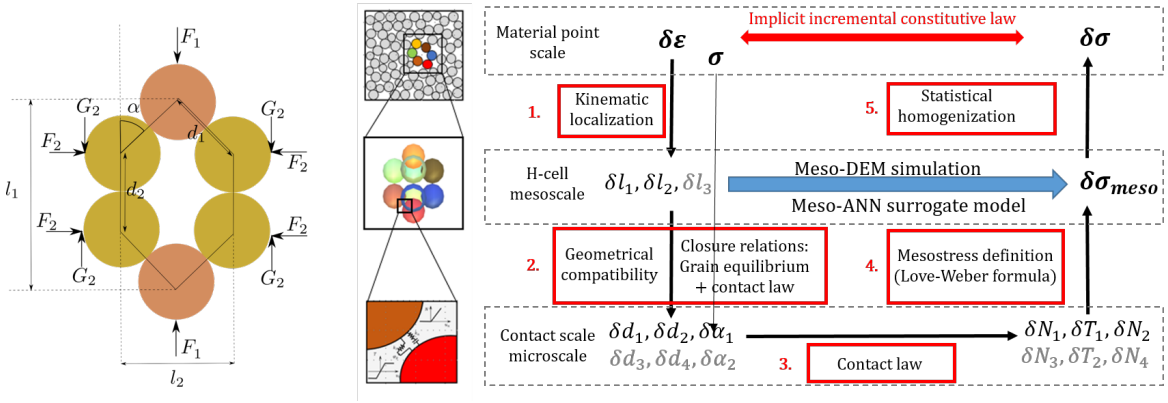

Figure 1. The H-cell (left) and the homogenization scheme for the standard H-model highlighting the integration of meso-DEM and meso-ANN strategies (right).

2. Meso-DEM strategy

Using the open source software YADE, the DEM model of the 2D H-cell can be proposed by using spheres of equal radii in interactions through linear elasto-frictionnal contact laws. To conform to the hypotheses of the original H-model, the degrees of freedom in rotation are blocked, the ratcheting correction terms are disabled and strain control is imposed by controlling the grain velocities. For grains of a unit size (1 m), the contact parameters consist of a normal stiffness $k_n = 2.10^8$ (N/m), a tangential stiffness $k_t = 0.5k_n$ and a friction angle $\phi_g = 30°$. After benchmarking the DEM response of a single H-cell against the analytical expression of the H-model [6, 7], the DEM based version of the H-model is constructed as follows:

1. Define a common macroscopic strain increment $\delta\epsilon_{macro}$ for all H-cells ;
2. Pass $\delta\epsilon_{macro}$ to a distribution of H-cells of different orientations with respect to the macroscopic frame. The same $\delta\epsilon_{macro}$ generate different incremental changes in the geometry of the H-cells depending on their orientation ;
3. For each H-cell direction, load the previous configuration in YADE and run a DEM simulation to update the geometry. Save the new H-cell configuration and return the different meso-stresses according to the Love-Weber formula ;
4. Compute the macro-stress as a statistical average of all meso-stresses. The weights are taken equal if the initial microstructure is isotropic.

Such a meso-DEM approach resembles to standard DEMxFEM approaches [9] except that it relies on several DEM simulations of a few grains (that run easily in parallel) compared to a single REV scale DEM simulation containing a much larger number of grains.

3. Meso-ANN strategy

Instead of running DEM simulations for several mesostructures at each strain increment, an alternative strategy consists in using the DEM to explore the accessible mesostructure configurations (geometry and contact forces) and construct a learning database by probing the incremental response for many strain increments. These offline DEM computations are used to train an artificial neuron network (ANN) that is used instead of the DEM in the homogenization scheme of Figure 1. Applying machine learning at the mesoscale is interesting for two reasons: the construction of the learning database relies of very fast simulations, and we can take out of the machine learning process as much physics as possible (e.g., the strain homogeneity and statistical homogenization steps).

To explore the accessible mesostructure configurations, we propose to follow proportional loading paths for different initial opening angle of the H-cell. Then, for sampled configurations, we impose incremental strain probes to get the incremental behavior of the H-cells. By doing so, we construct a learning database with 3.10^5 data points.

The construction of the ANN for the learning process is illustrated in Figure 2, where the input parameters are computed during the proportional loading step (in blue) or during the incremental strain probing step (in red).

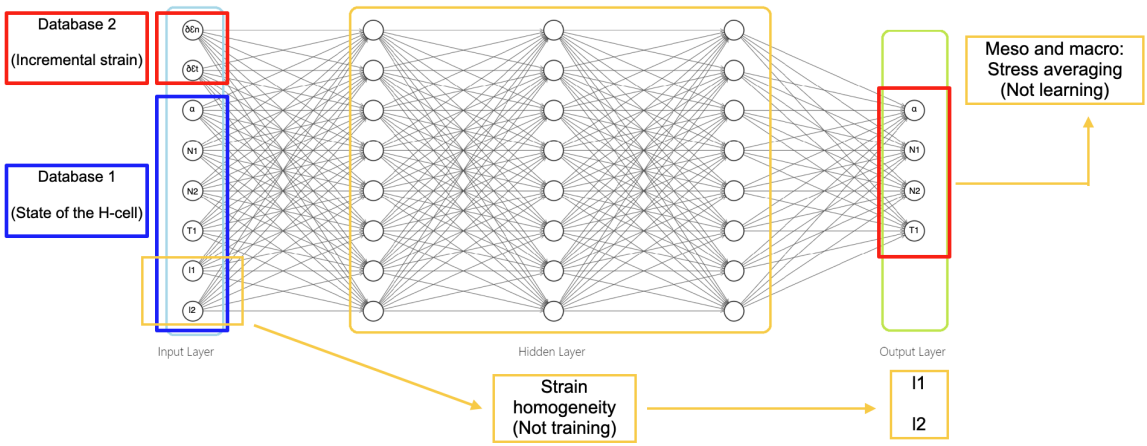

Figure 2. Architecture of the ANN used to learn the mesoscale behavior of the H-cell.

After testing several ANN architectures, normalization methods and loss functions, we have selected an ANN with three hidden layers of eight nodes, a hyperbolic tangent activation function, the z-score normalization method and the mean square error (MSE) loss function. The learning database was cured from pathological geometrical configuration, normalized by dividing lengths and forces by the grain diameter and the grain diameter times the contact stiffness respectively, and split into training and validation sets in respective proportions 0.8 and 0.2.

4. Benchmark against analytical H-model

To validate the meso-DEM and meso-ANN versions of the H-model, we conducted constant volume biaxial tests and benchmarked the predictions against the original analytical version of the H-model. Figure 3 show the results of the three models in the Cambridge plane.

Figure 3 highlights that all models give very similar results, which validates the construction of the meso-DEM and meso-ANN versions of the H-model. The ANN-model is completely superposed with the original analytical model while there is a slight discrepancy observed in the results from the DEM model. This is related to the implementation of the strain control in YADE during the isotropic compression step, which did not enable to reach the prescribed p with the same precision as for the analytical model. It is remarkable to highlight that the three H-models are able to account for the static liquefaction observed for loose material during constant volume biaxial test.

5. Perspectives

The use of meso-DEM simulations directly in multi-scale modeling and for constructing learning data bases opens promising perspectives for the development of multi-scale models relying on complex mesostructures for which no analytical relation exists to describe their mechanical behavior. In particular, when considering widely graded materials with varying fine contents (as it is the case

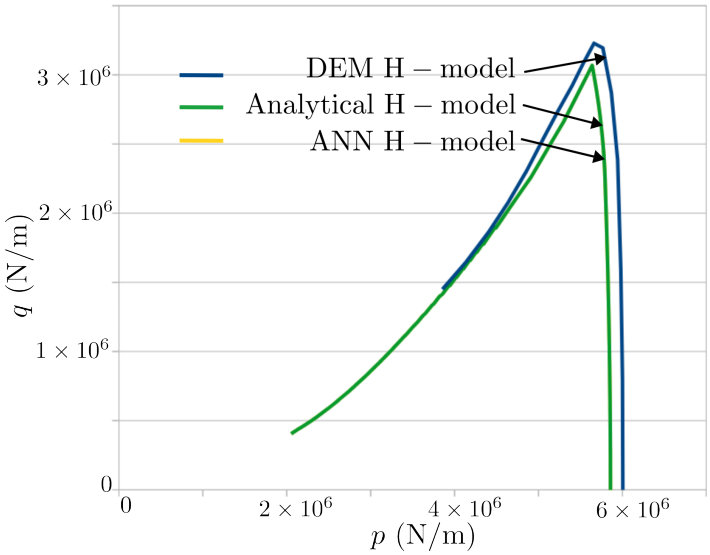

Figure 3. Comparison between the mechanical responses of the meso-DEM and meso-ANN models against the original analytical H-model for a constant volume biaxial test. The initial opening angle used in all models is $\alpha = 55°$. Deviatoric stress q and mean pressure p are expressed in 2D conditions.

for materials subjected to internal erosion or filtration processes) a 3D H-cell with fine grains included in the pore space can be used in meso-DEM or meso-ANN enriched version of the H-model [10].

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