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Multi-scale modelling of granular pile collapse by using material point method and discrete element method

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Abstract

Granular debris flows are often observed in mountainous areas in Southwestern China. The process is accompanied with large deformation and the evident transitions between solid- and fluid-like states bring difficulties in proposing a unified phenomenological constitutive model. In this study, a hierarchical multi-scale modelling scheme is developed, and is applied to simulate a granular pile collapse. The macroscopic behavior is modelled by using material point method (MPM), which is suitable for large deformation treatment, while the constitution relation at each material point is extracted from discrete element method (DEM) modelling. This MPM/DEM multi-scale modelling strategy abandons any constitutive assumptions as required in MPM, and facilitates effective cross-scale interpretation and understanding of granular flow behavior. It provides a potential approach to simulate large deformation of granular materials when their constitute relations are hard to be derived explicitly.

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Keywords: material point method; discrete element method; multi-scale modelling.

1. Introduction

Granular materials are important constituents in many industrial processes and geophysical phenomena. Understanding the evolution of internal structures of granular flows would certainly be of considerable helps when describing and predicting natural geophysical hazards, particularly the frequent granular-type debris flows that occur in the mountainous areas of Southwestern China [1]. Within the framework of continuum mechanics, it is hard to establish a unified constitutive model for granular media because they can behave like solids or fluids [2]. Various phenomenological parameters would also be introduced with no physical meaning or difficult to calculate [3]. Discrete element method (DEM) tracks all individual particles within their discrete nature, providing rich information at the microscopic level of the granular material. Since all the particles are modeled in their real sizes, the simulation time is consuming and it is currently unrealistic for DEM to model real engineering.

Clearly, investigating the mechanical behaviors of granular material from the microscale and macroscale views respectively are on two distinct modeling approaches. Multiscale modelling approach provides a feasible solution

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to fully utilize the advantages of these two methods. There are approximately three main schemes for multiscale modelling. Firstly, we extract the kinematics of grains from DEM to continuum mechanics, such as the evolution of frictional resistance and dilatancy (or internal plastic variables), which are known to be key variables in the macroscopic description of granular materials. Note that a phenomenological model is still needed in this solution [4]. Secondly, bridging scale method decomposes the computational domain into the coarse region and the fine scale region. The previous region covering the whole medium is simulated with FEM, while the later region limited to a localized zone is numerically simulated with DEM. The displacements of particles are interpolated into the nodes of FEM and a layer of virtual interfacial particles in the macroscopic region are assumedly generated to impose the interfacial condition applied to the DEM region [5,6]. Thus, the realistic mechanical responses, particularly the progressive localized failure process, and the micro-structure evolutions can be captured using less unknown variables than modelling with DEM. Recently, a new hierarchical multiscale technique has been proposed. In this strategy, the boundary value problem is solved by FEM on the macroscale, whereas the constitution relation is derived from DEM modelling at each integration point of the FEM [3,7].

Considering that FEM is difficult to model behaviors involving large deformations due to mesh distortion, we extend the hierarchy multiscale modelling scheme using MPM and DEM. The paper is organized as follows. The next section presents the details of modelling scheme including algorithms of both MPM and DEM, and the coupling method of MPM and DEM. By using the MPM/DEM method, Section 3 shows the simulated example of the collapse process of a granular pile . The summary is given in Section 4.

2. Modelling scheme

As shown in figure 1, MPM is used for macroscale modelling and DEM is adopted for microscale modelling. Each material point is a representative volume element (RVE) consisting of granular packing. The deformation information obtained by MPM is applied to the RVE as boundary conditions, while the Cauchy's stress calculated by DEM is reflected to MPM for the next step.

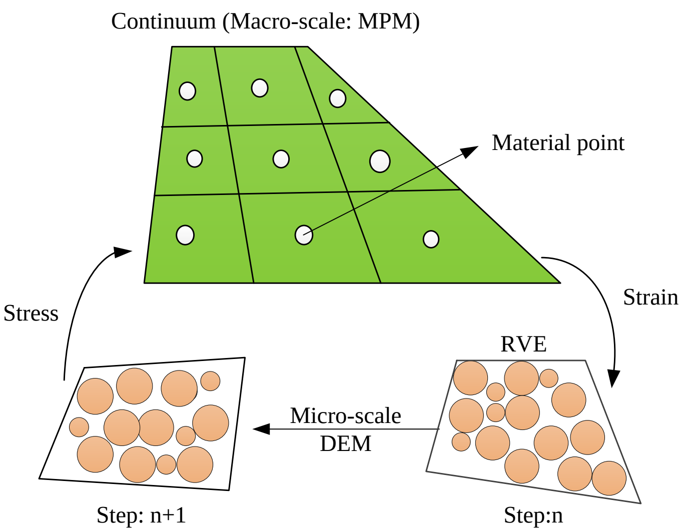

Fig. 1. Schematic of hierarchy multiscale modelling scheme.

2.1. *Algorithm of MPM*

MPM, as a mesh-free method, combines the Lagrangian description and Eulerian description. As shown in figure 2, (a) the material points carrying all the physical variables, such as mass and momentum, are linked with the background grid, (b) according the second law of Newton, the grid nodes update their positions and other kinetics, (c) these updated information of nodes are interpolated to the material points, and (d) in the next step, a new mesh would be adopted.

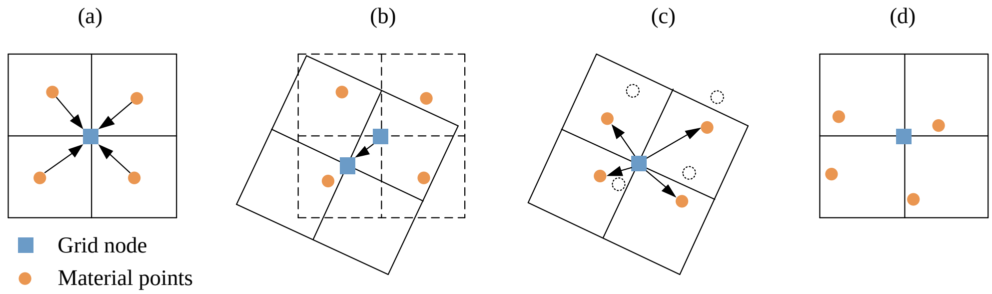

Fig. 2. Calculation procedure of MPM.

The governing equations are mass conservation, balance of momentum, and conservation of energy. As the mass is carried by the material points, the conservation of mass is automatically satisfied. Meanwhile, the energy balance can afterwards be used as an auxiliary equation to estimate the accuracy of the model [8]. The motion of material points only governed by the conservation of momentum that implies that:

$$\rho \dot{v}_i = \sigma_{ij,j} + \rho b_i \tag{1}$$

where, ρ is the current density, $\dot{v}_i$ is the acceleration vector, a dot notation indicates differentiation with respect to time, $\sigma_{ij,j}$ is the spatial gradient of stress tensor, b_i is the specific body force. The weak form of equation (1) is written as:

$$\int_{\Omega} \rho w_i \dot{v}_i d\Omega = \int_{\delta\Omega_\tau} w_i \tau_i dS - \int_{\Omega} w_{i,j} \sigma_{ij} d\Omega + \int_{\Omega} \rho w_i b_i d\Omega \tag{2}$$

where Ω is the study region, $\delta\Omega_\tau$ is the stress boundary, w_i is an arbitrary test function, $\tau_i = \sigma_{ij} n_j$ is the surface traction, and n_i is the outward unit vector. In the generalized interpolation material point method (GIMP), particles are defined by "particle characteristic functions", $\chi_p(x)$, which represents the space occupied by a given particle, and can be thought of as the spatially varying volume fraction of that particle [9]. Given a material point property, f_p, a representation consistent with the initial discretization procedure is the sum over the material points,

$$f(x) = \sum_p f_p \chi_p(x) \tag{3}$$

Here, the nodal shape functions are used to represent the field of admissible test functions:

$$w_i(x,t) = \sum_I N_I(x) w_{iI}(t) \tag{4}$$

where $N_I(x)$ is the nodal shape function associated with node I. Substituting equations (3) and (4) into equation (2) and utilizing that the test functions are arbitrary, we can get the following governing equations:

$$\begin{aligned} \sum_p \frac{\dot{p}_{ip}}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(x_i) N_I(x_i) d\Omega = &- \sum_p \sigma_{ijp} \int_{\Omega_p \cap \Omega} \chi_p(x_i) N_{I,j}(x_i) d\Omega \\ &+ \sum_p \frac{m_p}{V_p} b_{ip} \int_{\Omega_p \cap \Omega} \chi_p(x_i) N_I(x_i) d\Omega + \int_{\delta\Omega_\tau} N_I(x_i) \tau_i(x_i) dS \end{aligned} \tag{5}$$

where, Ω_p is the volume of material point p, $\dot{p}_{ip} = m_p \dot{v}_{ip}$ is the material time derivative of the momentum. Introducing the weighting function and its gradient as:

$$S_{Ip} = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(x_i) N_I(x_i) d\Omega, \quad S_{Ip,j} = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(x_i) N_{I,j}(x_i) d\Omega \tag{6}$$

respectively, yields the discrete equation:

$$\dot{p}_{iI} = f_{iI}^{\text{int}} + f_{iI}^{\text{ext}} \tag{7}$$

where $\dot{p}_{iI}$ is the rate of change of the total momentum, f_{iI}^{int} is the vector of interal force and f_{iI}^{ext} is the vector of external force, which are defined as:

$$\dot{p}_{iI} = \sum_{p} \dot{p}_{ip} S_{Ip} \tag{8}$$

$$f_{iI}^{\text{int}} = -\sum_{p} \sigma_{ijp} S_{Ip.j} V_P \tag{9}$$

$$f_{iI}^{\text{ext}} = \sum_{p} m_p b_{ip} S_{Ip} + \int_{\delta\Omega_\tau} N_I(x_i)\, \tau_i(x_i) dS \tag{10}$$

Summarily, the momentum of grid node can be updated by:

$$p_{iI}^{\text{n+1}} = p_{iI}^{\text{n}} + f_{iI}^{\text{total,n}} \Delta t \tag{11}$$

where, subscripts n + 1 and n mean iterative steps, and Δt is the time step. Once the grid update is done, these results are used to update particle velocity and position.

$$v_{ip}^{\text{n+1}} = v_{ip}^{\text{n}} + \Delta t \sum_{I} a_{iI}^{\text{n}} S_{Ip}^{\text{n}}, \quad x_{ip}^{\text{n+1}} = x_{ip}^{\text{n}} + \Delta t \sum_{I} v_{iI}^{\text{n+1}} S_{Ip}^{\text{n}} \tag{12}$$

Since the stress is updated by RVE, no constitutive model is needed in MPM.

2.2. Algorithm of DEM

In DEM, particles interact with others through contacts. Many types of contacts laws have been proposed to deal with various behaviors, such as capillary phenomenon. However, in this work, we focus on the framework of multi-scale modeling using DEM and MPM, rather than on the complicated interaction mechanism between particles. Therefore, the simplest linear contact law with damping is adopted to calculate contact forces. As shown in figure 3, for particle 1, the position vector is $\mathbf{OO_1}$, the linear velocity is $\mathbf{v_1}$, the angular velocity is $\omega_\mathbf{1}$, and the radius is R_1. Identical notation is adapted for particle 2. If the distance between particle 1 and particle 2 is smaller than the sum of their radius, a contact would be detected, and the overlap of this contact is defined as:

$$\delta = R_1 + R_2 - |\mathbf{OO_1}| \tag{13}$$

where, $|\cdots|$ denotes the length of vector. The normal vector of contact is aligned the line connecting the centers of particles, e.g. $\mathbf{n} = \mathbf{O_1O_2} / |\mathbf{O_1O_2}|$, and the tangential vector is perpendicular to the normal vector. The contact point C is assumed locating at the middle of the contact, whose location vector is:

$$\mathbf{OC} = \mathbf{OO_1} + \frac{\mathbf{1}}{\mathbf{2}} \left((R_I - R_2 + |\mathbf{O_1O_2}|) \mathbf{n} \right) \tag{14}$$

Thus, the relative velocity of particle 1 and particle 2 at point C is:

$$\Delta\mathbf{v^c} = \mathbf{v_1^c} - \mathbf{v_2^c} = \mathbf{v_1} - \mathbf{v_2} + \omega_\mathbf{1} \times R_I \mathbf{n} + \omega_\mathbf{2} \times R_2 \mathbf{n} \tag{15}$$

The contact force along normal direction is computed as:

$$f_\text{n} = k_n \delta - \eta_n \Delta\mathbf{v^c} \cdot \mathbf{n} \tag{16}$$

where, k_n is the coefficient of normal stiffness of contact, and η_n is the damping coefficient in normal direction. For the tangential direction, Coulomb friction law is adapted, and the tangential contact force can be obtained by:

$$f_t = \min\left(k_s (\Delta\mathbf{v^c} \cdot \mathbf{t}) \Delta t - \eta_s \Delta\mathbf{v^c} \cdot \mathbf{t},\ \mu_s f_n \right) \tag{17}$$

where, k_s is the coefficient of shear stiffness of contact, Δt is the time step, η_s is the damping coefficient in tangent direction, and μ_s is the frictional coefficient.

Summarily, the contact force and the torque exerted to the center of particle 1 are:

$$\mathbf{f} = f_n \mathbf{n} + f_s \mathbf{t}, \quad \mathbf{M} = R_1 \mathbf{n} \times f_s \mathbf{t} \tag{18}$$

respectively. Thus, the location and rotation of particle 1 would be updated by Newton's equation of motion.

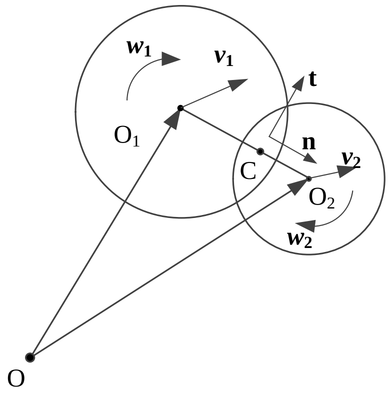

Fig. 3. Schematic of contact in DEM.

2.3. MPM/DEM coupling

Detail information of granular packing, such as local structures and contact forces, can be obtained by DEM, while the macroscopic information, such as deformation of RVE, is achieved by MPM. In the multi-scale modelling scheme, the deformation of material point is equivalently applied into the RVE through boundary conditions. Thus, particles would arrange to resist this deformation, leading to the change of configuration of granular contacts. Macroscopic Cauchy's stress is linked with the contact forces as:

$$\sigma_{ij} = \frac{\phi}{\sum_{N_p} V_p} \sum_{N_p} \sum_{N_c} \left| x_i^c - x_i^p \right| n_i^{c,p} F_j^c \tag{19}$$

where, ϕ is the volume fraction, N_p is the number of particles in a RVE, V_p is the volume of particle p, N_c is the number of contacts, x_i^c is the position vector of contact point c, x_i^p is the central position of particle p, n_i^{cp} is the contact normal direction, and F_j^c is the contact force vector at point c. The microscopic information is transformed into macroscopic analysis. Note that, unlike DEM, no stiffness matrix is needed in MPM. From equation (19), it can be seen that the number of particles in a RVE is essential for the calculation of Cauchy's stress. In the reference [3], researchers examined the anisotropy of coordination number of RVE under isotropic loading, and found that at least 400 particles in 2-dimensional RVE is acceptable. As shown in figure 4, in this work, a RVE contains 900 particles to satisfy the need for large deformation analysis. Periodic boundary conditions are applied in all directions to satisfy mass conservation. The radius of particles uniformly distributes between 3 mm and 7 mm to avoid crystallization. Similar to previous study [3], the material parameters used for particles are listed in below: density is 2650 kg/m^3; Young's modulus and Poisson's ratio are 600 MPa and 0.8 respectively; Surface frictional coefficient is 0.5.

Fig. 4. A sample of the initial configuration of granular packing of a RVE.

3. Collapse of sand pile

The collapse of sand pile is chosen as an example to demonstrate the capacity of multi-scale modelling to describe the granular behaviors. Initially, particles are confined into a rectangular column using a plate. Then, granular flow would occur after the plate being removed. In the whole process, particles exhibit transitions of solid-like and fluid-like behaviors, and undergo large deformation. As shown in figure 5, in this work, the confined region is 10 cm × 20cm, and the size of background cell is 1cm, which contains four material points initially. Thus total 800 material points are used to simulate the collapse process. Note that each material point accords to a RVE containing 900 particles. Gravity is applied along negative direction of y-axis with $g = 9.8\mathrm{m/s}^2$.

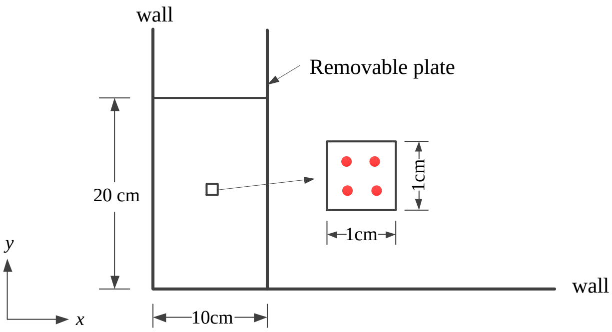

Fig. 5. Schematics of setup of the sand pile collapse in simulation.

Figure 6 shows the initial distribution of vertical stress and the force-chain networks in different locations. The right color legends dedicate the values of normal contact force. It can be found that the vertical stress increases with depth, as expected. In the microscopic view, stronger force chain is also found at bottom. Thus, to some extent, the hierarchy modelling scheme is efficient to describe solid-like behavior of granular media. After removing the plate, particles would flow down under gravity.

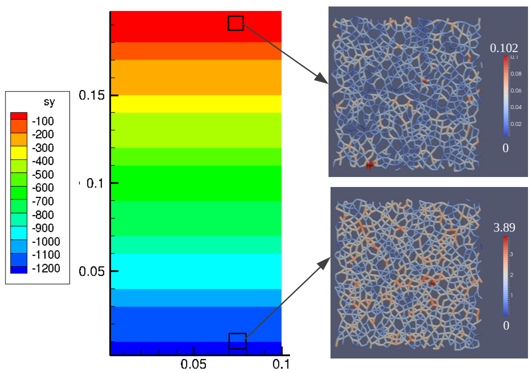

Fig. 6. Under gravity, the static packing is obtained at initial state. Left: distribution of vertical stress. Right: force-chain networks in a bottom material point and in a top material point.

Figure 7 shows the collapse process in terms of vertical displacement, in which large deformation is clearly observed. Pay attention to the final deposit configuration of sand pile. Since the red color denotes small displacement, a static zone like solid is found, while other region experiences granular flow. The solid-like and fluid-like behaviors of granular media are covered by this hierarchy modelling scheme. It should be reminded that no phenomenological constitutive model is assumed before, and the stress is extracted by RVE consisting of granular packing.

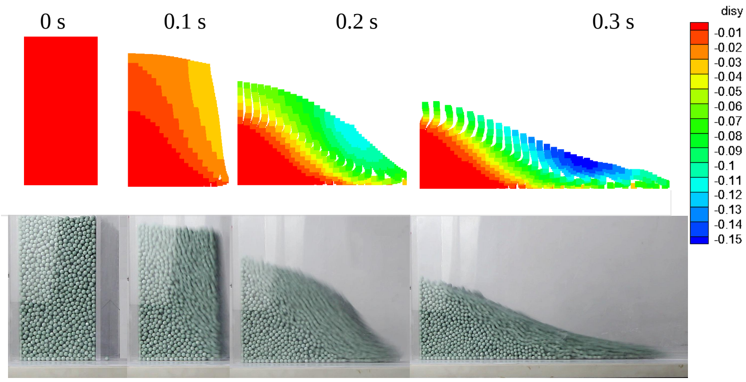

Fig. 7. Temporal evolution of distribution of vertical displacement of materials points in the collapse process and the experimental result.

4. Summary

This work establishes a new hierarchy multi-scale modelling scheme for granular materials. The macroscopic analysis is conducted by MPM, which is suitable for large deformation and large scale simulation, while the microscopic analysis is performed by using DEM, which provides details of packing information. Each material point is treated as a RVE, and is composed by a granular packing. Deformations of material points are applied into RVEs to reflect Cauchy's stresses, which is linked with contact forces. Without needing any phenomenological constitutive model, the process of collapse of sand pile is simulated with acceptable accuracy. This MPM/DEM modelling scheme extend the usage of previous FEM/DEM multi-scale modelling scheme to large deformation, and may provide a new method to study mechanics of the granular media.

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