Development of Advanced Particle Simulation Code

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1. Introduction

The Discrete element method (DEM) solves individual particle motions with contact frictions. Large-scale DEM calculations can reproduce the direct multiscale dynamics of collective motion of granular materials [1,2] and contribute to the development of truly physics-based geodynamics, disaster prevention and geotechnical applications. However, DEM is difficult to be parallelized especially in memory management of tangential forces. Therefore, we have developed the software DEPTH (DEM based Parallel mulTi-pHysics simulator) for large-scale parallel computing utilizing our original dynamic load balancing technique [3]. Here we report on the technological developments of DEPTH, such as the extension of particle interaction and the applications for the deep-sea mining, concrete flow, and geological scale rock-deformation.

2. Granular analysis of underwater mixing process

Mixing process is essential for handling granular materials in various fields. Recently, it has attracted attention for the potential usage for retracting mineral resources from undersea soils [4]. We extended and applied DEPTH for the design and optimization of mixing apparatus for underwater mixing [4,5,6]. In previous studies, we focused on calibration [4] and on the influence of geometrical and operational factors affected the mixing process [5]. In the paper [6] published in this FY, we investigated the influence of DEM parameters for an underwater mixing process (Fig. 1). Our model deals with typical contacting interactions and lubrication force to simulate the different kinds of soils.

Based on the calibrated and optimized settings from a previous study [5], we consider the changes in the target soils by conducted parametric study on the Young's modulus (E), Poisson's ratio (ν), coefficient of restitution (e), coefficient of friction (μ), coefficient of rolling friction (μ_r) and fluid viscosity (η_f). From DEM simulations, we measured the torque on the mixing blade and the overall performance of mixing with an original nondimensional parameter, mixing resistance [5]. We found out that rolling friction is the most influential microscopic

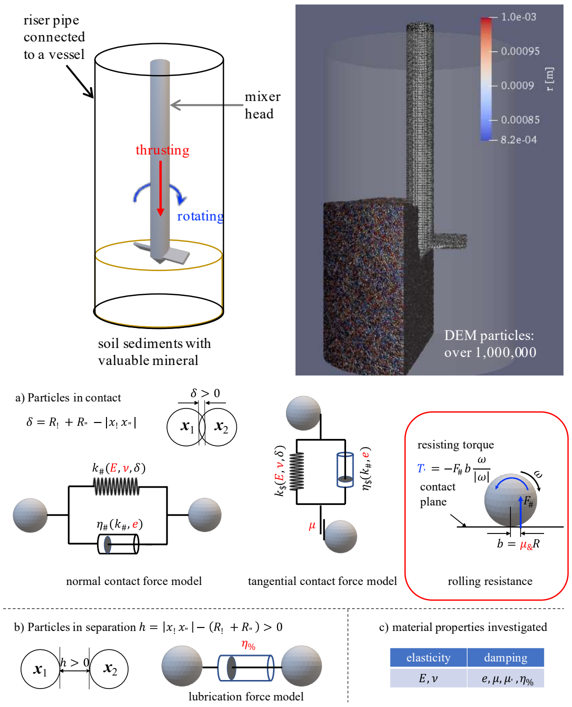

Figure 1: Upper left is illustration of mixing for deep sea and right is a corresponding 3D DEM simulation. Microscopic parameters for parametric study: (a)contact models; (b) lubrication; (c)role of parameters.

material parameter while the influence from the elastic moduli (E and ν) is negligible. Utilizing graph theory, we further revealed that the change in friction parameters alters the connectivity of stress chains which could explain the significant influence from rolling friction. The main findings are summarized in Fig. 2.
Fig. 2 Rolling friction (μ_r) exhibits the most significant influence on the torque response of the mixing process. A graph analysis of the stress chains reveal that the rolling friction influences the number of particles involved in the stress chains.

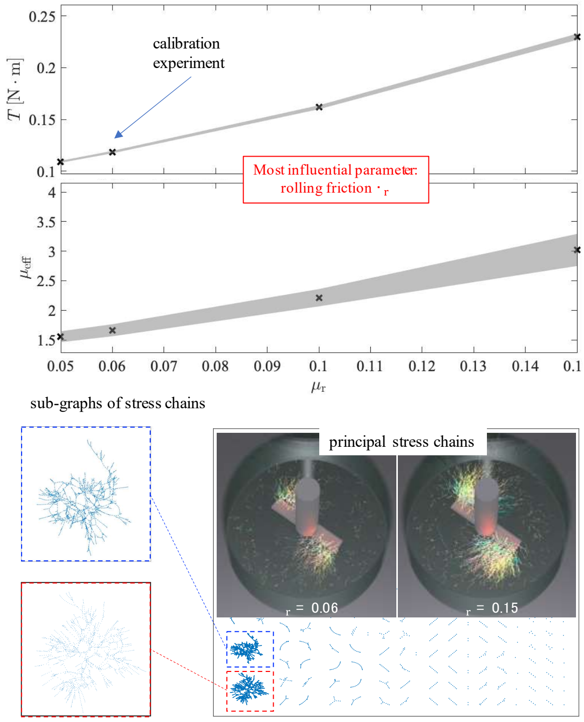

Figure 2: Upper panel is the influence of rolling friction. Lower panel is the graph analysis of the particles in the major stress chains from the two blades of the mixer head.

3. Development of viscoplastic flow model by DEM

To treat the large deformation of viscoplastic material such as grout and concrete, we develop the models of viscoplastic forces for DEPTH code. The viscoplastic model consists of plastic force F_{pla} and viscous force F_{vis} as follows:

$$F_{pla} = 2P_aMg[1/(1+P_bD^{I_b}) - 1/(1+P_bD^{I_a})] \quad (1)$$

$$F_{vis} = P_cMV \quad (2)$$

where $M = m_im_j / (m_i + m_j)$ with a particle mass m_i and m_j, and $D = S / E_{rad}$ with the distance S between particle surfaces and a range of viscoplastic forces E_{rad}, and V is the relative velocity between particles. P_a and P_c are main calibration parameters of actual material.

For example, grout or concrete are our target materials in the geotechnical engineering. To know the mechanical properties, some flow tests such as slump flow tests are performed. Thus, it is important to reproduce such experiment with DEM as shown in Fig. 3. Our model successfully reproduces the viscoplastic behavior of concrete.

Fig. 4 shows a practical application of the calibrated viscoplastic DEM model. We simulate the press-in behavior of grout material into reinforced concrete structures. This DEM application can be the digital twin of grout filling to the complicate reinforced concrete structures.

Figure 3: Slump flow test with DEM simulation for concrete.

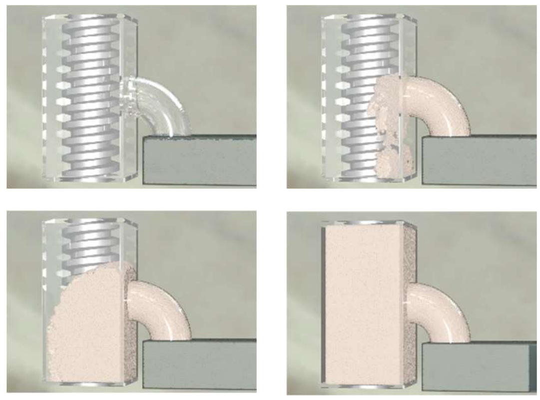

Figure 4: DEM simulation of press-in test of grout material.

4. The thrust formation with numerical granular rock box experiment

The numerical granular rock box experiment based on DEM is performed in the thin 3D geometry to investigate the role of granularity in the thrust formation. A numerical sandbox test has been extensively performed to study the stress state and formation of accretionary prisms [1]. The rock box experiment is an extension of the sandbox simulation with adhesive force. In the last FY, we develop the adhesion model which reproduces the triaxial compression test of the host rock of accretionary wedge.

With this model, we performed the numerical simulation of the horizontal shortening of a granular layer in the geological scale in this FY. The rock box test successfully reproduces the characteristic structures of accretionary wedge with the sequential thrust formations (Fig. 5).

Different from the analog sandbox test, the adhesion force generated the surface geometry with steeper angles, complex surface faults and enhanced bifurcation of the shear bands. The increasing complexity of the network was demonstrated with finer element until its maximum radius become 12.5 m with over 5 million particles (Fig. 6). We also analyze the granular nature

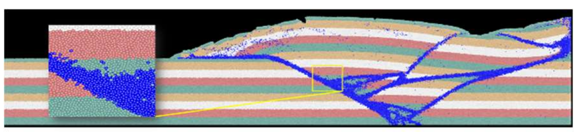

Figure 5: Snapshot of rock-box simulation with maximum radius 12.5 m for about 2 km thickness of the layer.

in the thrust thickness which depended on the number of frictional elements rather than the physical length. These results indicate important role of granularity in the evolution of the thrust.

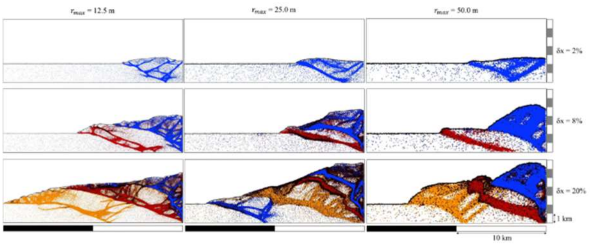

Figure 6: Difference by the element sizes. The colors (blue, red, and orange) show the generation of faulted materials.

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