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 regarding geodynamics, disaster prevention and geotechnical problems. However, the parallelization of DEM is technically challenging 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. In this project, we utilize and improve the DEPTH for various geodynamics, geotechnical and power engineering problems. Here, we introduce the achievements of this FY, regarding accretionary prism formation, land slide, and DEM model developments [1-4].

2. Thrust formation using a numerical granular rock box experiment

We performed 3D numerical simulations of a shortening granular rock layer at geologically relevant scales. The DEM interactions with the cohesive model imitate a failure envelope of the host rock in an accretionary wedge in the triaxial test. As shown in Fig. 1, the rock box simulation successfully demonstrated the sequential formation of thrusts. We found that models with cohesive forces generated clear precursors of thrust formation, surface geometries with steep angles, and vertical faults. The geometric network of fault planes depended on the healing of the cohesive force within the faulted region. The increasing complexity of the network was demonstrated using finer elements until its maximum radius reached 12.5 m. The size of the element was important for capturing such fine thrust structures. We also examined the potential role of granularity in the growth of the fault damage zone. We found that the width of the fault damage zone was controlled by the number of frictional elements rather than the physical length [1].

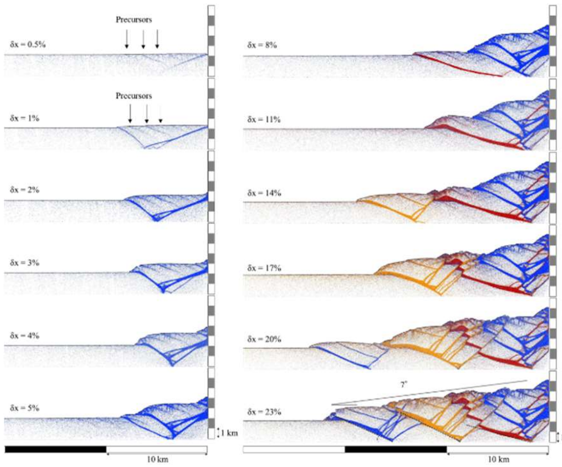

Figure 1: Evolution of the shortening layer with a granular fault model having maximum element radius 12.5 m. The faulted elements and surface of the layer are plotted for different shortenings δx. The color shows the period in which the elements are faulted.

3. Landslide simulation

Landslides are a major threat to human life and property. Numerical simulations can help to assess the landslide hazard and its impact on critical infrastructure. We aims to develop large scale DEM landslide simulations based on the DEPTH code to contribute to both the studies of landslide and better landslide hazard assessment. This can be achieved by a combination of large-scale simulation (i.e., high spatial resolution) and a well-controlled slope modeling technique.

This fiscal year, we applied a periodic granular (PG) box method developed in previous years to study the Aso Bridge landslide caused by the 2016 Kumamoto earthquake. Our main simulation results, summarized in Figures 2 to 4, have been published as a peer-reviewed international journal paper [2]. A major advance of this study over the existing literature is that the slope is excavatable, i.e., surface materials can be removed and entrained by the initially released geomasses, see Figure 2. We also found that the runout distance depends on the particle size and that smaller particles lead to a landslide with a longer runout distance, see Fig. 3. Analysis of individual particles showed that the difference in runout is due to the maximum travel distance of the particles and the frequency of particles with a given travel distance, see Fig. 4. This implies that a granular system of small particles is more mobile than a granular system of large particles. The mechanisms underlying this observation require further study. More details of the study can be found in the paper [2].

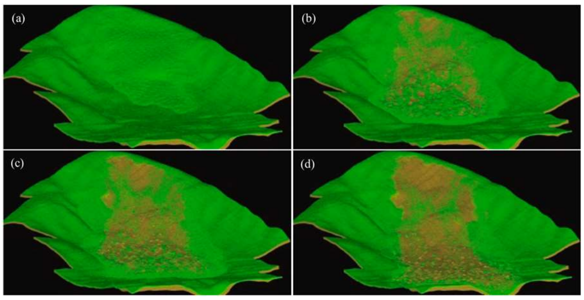

Figure 2 Landslide simulation of the Aso Bridge landslide: the removal and entrainment of surface materials are visible.

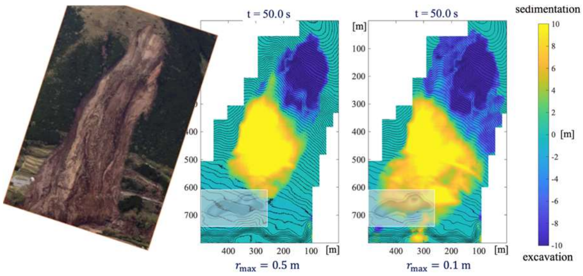

Figure 3 Particle-size dependent runout distance in DEM landslide simulations.

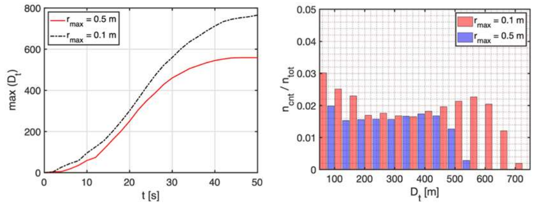

Figure 4 Left: Maximal particle travel distance D_{t}; Right: frequency of particle counts $n_{\mathrm{cnt}}/n_{\mathrm{tot}}$ with a certain D_{t}.

4. JKR theory-based force model for adhesive contact

Adhesive particles are common in nature and industry. DEM simulations of adhesive particles require well-founded force models. On the one hand, contact theories, such as the JKR theory, have shown very good agreement with contact experiments. On the other hand, contact theories focus on predicting the contact size caused by an applied force, while for DEM simulations the contact force must be evaluated from their relative displacement. Unfortunately, due to the complexity of contact theories involving surface energy, it is difficult to derive an analytical relationship between force and displacement for adhesive contact, see Fig. 5.

In this fiscal year, we successfully derived an analytical force-displacement relation from the JKR contact theory, and the results were published as an international journal paper [3]. As shown in Figure 6, we not only obtained a JKR force model from our derivation, but also extended it to a smoothed JKR (sJKR) model. Our sJKR model is characterized by a smooth evolution of the force when a contact is made or broken, see Fig. 6. This feature leads to easier implementation and stable integration [3]. We compared the two models with a bouncing ball simulation, in which the ball is dropped over an infinite surface and then undergoes the cycles of contacting and leaving the surface. As shown in Figure 7, the original JKR is dissipative for every separation, even when no explicit damping is introduced in the simulation. In contrast, the sJKR model is energy-conserving without external damping. More details can be found in our paper [3].

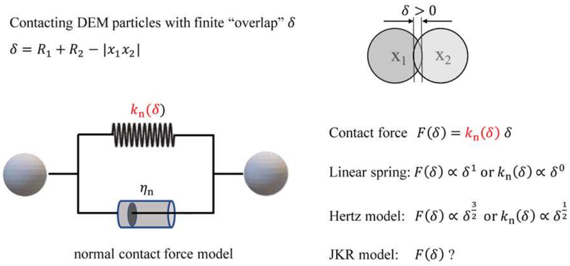

Figure 5 Analytical force-displacement relation is needed for efficient DEM simulations of adhesive particles.

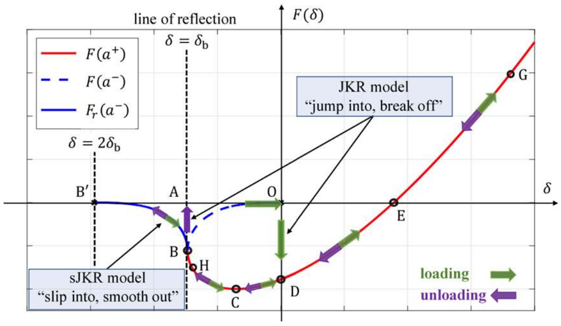

Figure 6 Analytical force-displacement relation is obtained from JKR theory (i.e., JKR model) and is extended to a smoothed JKR (sJKR) model.

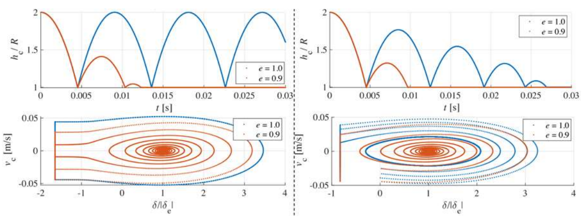

Figure 7 Simulation of a bouncing ball using the smoothed JKR model (left) and the original JKR model (right) under two different nominal restitution coefficients $e = 0.9, 1.0$.

5. Performance and feature improvement of DEPTH

In this FY, we improve the capabilities of DEPTH. To deal with multiphase flow, we implement the new fluid flow solver and coupling modules to DEPTH. In addition, we implemented the advanced boundary modules to enable flexible handling of moving (deforming) structures given by the CAD data. This new module is available not only for granular material but also the fluid.

In the coupling of DEM and fluid calculations, the fluid calculation part was implemented using particle-based Smoothed Particle Hydrodynamics (SPH) and grid-based Computational Fluid Dynamics (CFD). SPH was implemented with the same parallelization techniques as those used in DEM. For the pressure Poisson equation in CFD, we employed the parallelized Multigrid solver with SOR method. For the interaction model between granular materials and fluids, we used a local averaging model that estimates the fluid resistance force from local average physical quantities.

Regarding the movement of structures, we computed the rigid body motion based on the interaction forces among structures and between structures, granular materials, and fluids. The interaction forces between structures, and between structures and granular materials, were calculated using a signed distance function. The interactions between structures and fluids in CFD were determined through direct numerical calculations using an embedded boundary method, while in SPH, they were determined through interaction calculations with SPH particles attached to the structures.

Figure 8 present the results of inserting and pulling out an anchor into the ground made of granular material. When the anchor is pulled out, we successfully reproduced the opening of the fixture at the tip of the anchor due to the influence of the ground particles. The geometry of the anchor was generated by the new modules from the CAD data.

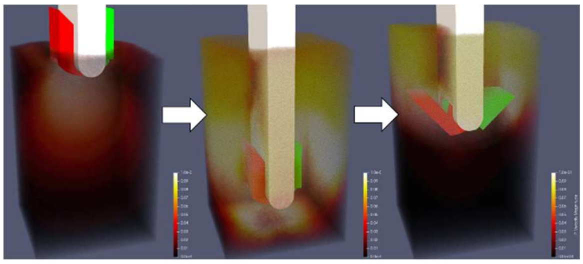

Figure 8: Simulation of anchor inserted into the ground.

Here we present the results of coupled simulations of DEM-CFD (Fig. 9) and DEM-SPH (Fig. 10). In the DEM-CFD simulation of Fig. 9, we conducted a multiphase flow simulation of air and granular materials, and it was possible to confirm that fluid flow occurs due to the influence of granular materials and structures. On the other hand, in the DEM-SPH simulation of Fig. 10, we carried out a multiphase flow simulation of water and granular materials, making it possible to examine the impact of water flow on the motion of the granular materials.

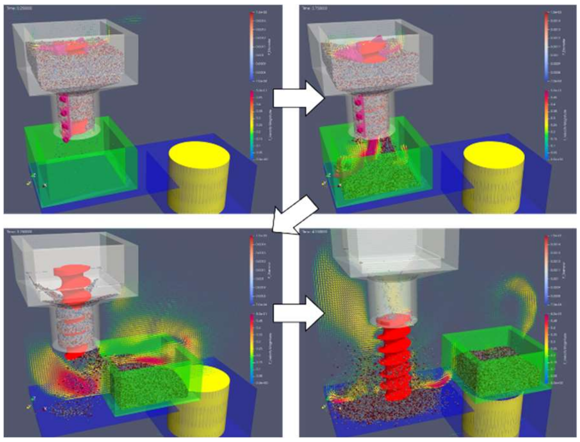

Figure 9: Coupled Simulation result with DEM-CFD model

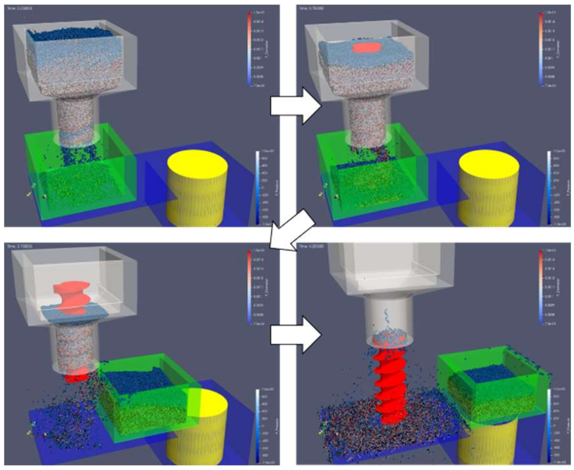

Figure 10: Coupled Simulation result with DEM-SPH method

To improve the performance of particle simulation method, we also investigate the utilization of lower precision including half precision. However, improving HPC performance at such low-order precisions is a challenge. An as-is implementation with half-precision will have lower computational cost than that of float/double precision simulations, but also worsens the simulation accuracy. We propose mixed precision approach with a scaling and shifting method that maintains the simulation accuracy near the level of float/double precision. By examining the simulation accuracy and time-to-solution, we demonstrated that the use of half-precision can improve the computational performance of SPH simulations for scientific purposes without sacrificing the accuracy [4].

Acknowledgement

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Science (JSPS).

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