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 directly reproduce the multiscale dynamics of collective motion of granular materials regarding geodynamics, disaster prevention and geotechnical problems. The parallelization of DEM is technically challenging especially for the efficient data management of tangential forces in both shared and distributed memory system. 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 the earthquake, accretionary prism formation, and DEM model developments [1-4].

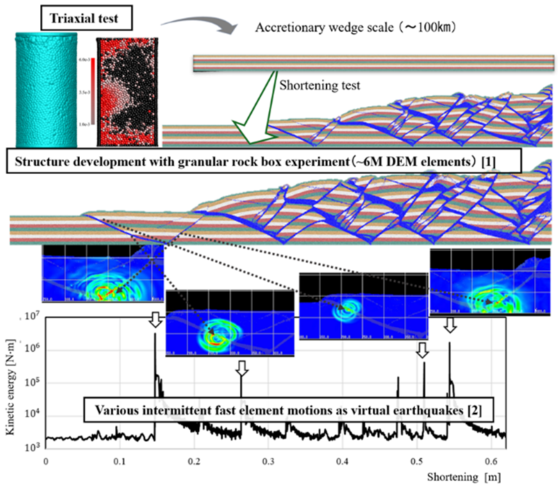

Figure 1: Flow of the granular rock box simulation: triaxial compression test, fast convergence test for structural development, and slow convergence test to analyze seismic events.

2. Virtual earthquakes in a numerical granular rock box experiment

We developed a virtual earthquake simulation using a numerical granular rock box experiment, an extension of the numerical sandbox test that incorporates cohesive contact forces. Our model simulates the horizontal shortening of a thin 3D granular rock layer, spanning 100 km with periodic boundary conditions, using about seven million DEM elements (maximum radius of 12.5 m) on the Earth Simulator.

To imitate realistic rock failure behavior, we first performed a triaxial compression test on the granular media with the cohesive model. We then conducted a fast convergence test on a flat granular layer to simulate sequential thrust formation, similar to an accretionary wedge [1]. Finally, we perform a slow convergence test to reproduce intermittent fast motions along faults that generate waves, which is interpreted as virtual earthquakes [2]. These results demonstrate that the granular rock box simulation seamlessly reproduces both seismological and geological-scale processes (Fig. 1).

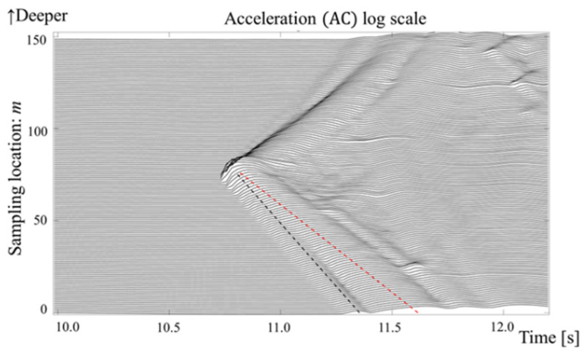

Figure 2: Wave propagation along the fault. The red and black dashed lines show propagations with 2.6 km/s (fracture) and 3.7 km/s (p-wave), respectively

The hypocenter, which is not predefined in our model, emerges within the active fault damage zone and shifts as the geological structure evolves. Seismic events occur when the fault undergoes shear motion, characterized by 3D element-wise rotation and double-couple behavior, and they follow the Gutenberg–Richter law. The fracture propagation speed is approximately 2.6 km/s, and additional wave velocities of about 3.7 and 2.7 km/s likely correspond to P-waves and S-waves, respectively (Fig. 2). Furthermore, the slip distance and mean stress drop at the hypocenter are around 1.8 cm and 0.46 MPa, and the dominant wave frequency is 3–4 Hz. These findings demonstrate the feasibility of granular rock box simulations for reproducing realistic, multiscale mechanisms that bridge seismological and geological phenomena.

3. Numerical investigation on fault vergence

Most of the Earth's earthquakes occur at the margins of subduction zones, where oceanic plates subduct beneath continental plates, occasionally triggering destructive tsunamis. The lateral segmentation of earthquakes along the Sumatra subduction zone is well documented. However, the significant variability in seismic behavior between segments suggests that local structures play a critical role in controlling coseismic slip propagation. In particular, structures within frontal accretionary prisms are strongly associated with tsunami generation. A better understanding of the formation of frontal prism structures can contribute to assessing seismic-induced tsunami hazards in the Sumatra subduction zone and elsewhere.

To investigate the evolution and controlling factors of local deformation structures in the frontal accretionary prism, in particular fault vergence, we performed numerical sandbox experiments using the Discrete Element Method (DEM), in particular the DEPTH code parallelized on ES. Our numerical sandbox is shown in Figure 3. The shortening of a sedimented layer of granular particles is used to model rock deformation in a subduction process. The shortening is achieved in the simulation by pushing a backstop wall against the sediment layer, which is equivalent to pulling the layer against a fixed backstop. The dip angle is adjustable in our DEM modeling, and we chose a fixed value of 4°to be consistent with the field observations [3].

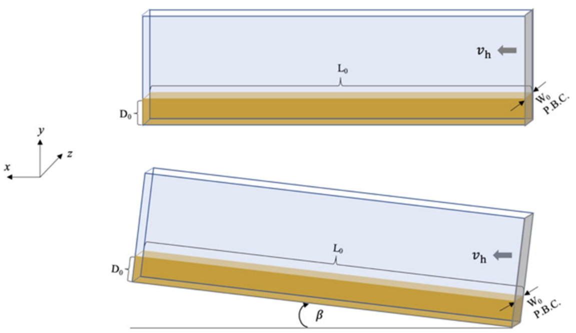

Figure 3: Numerical sandbox for studying fault formation.

The simulation results of the numerical sandbox experiments at different shortening stages are shown in Fig. 4. From this figure, we can see the influence of the basal friction μ_b on the local structure formation under fixed interparticle friction μ_p. With a low μ_b = 0.02, only landward vergent folds and bivergent folds were initially formed. As μ_b increased to 0.05 and 0.1, the number of bivergent folds increased, while the number of landward vergent folds decreased. As μ_b increased to 0.2, the landward vergent fold disappeared, and the seaward vergent folds appeared.

Besides the influence of basal friction, we also investigated the influence of interparticle friction. We found that the influence of interparticle friction mainly affects the spatial extent of folds, but not the type of folds. We concluded that in terms of friction, basal friction is the main control of fault vergence. The spatial variation in fault vergence may correspond to a variation in basal friction in the Sumatra subduction zone. More details can be found in our publication [3].

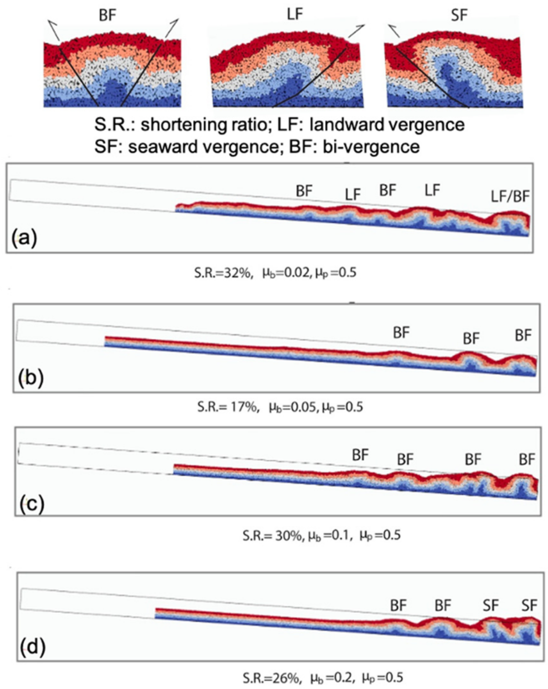

Figure 4: Influence of basal friction on fault vergence: for a fixed interparticle friction μ_p = 0.5, the basal friction is varied to study its influence on the vergence.

4. Compression of Hierarchical Granular Piles

Hierarchical granular piles (HGPs) composed of aggregates are key structural features in both geoscience and planetary science, from fault gouge in seismic zones to the internal structures of comets. The compressive behavior of HGPs has been investigated primarily through experimental studies. These studies have reported that the packing structure of HGPs evolves during compression in a multi-step process. Under low confining pressure, the deformation is characterized by the rotation of aggregates, whereas under high confining pressure, aggregate breakage drives structural evolution. Furthermore, deformation of constituent particles occurs when the applied pressure is sufficiently high.

In this fiscal year, we performed DEM simulations of the compression behavior of HGPs (Fig. 5). We analyzed the compressive behavior of these piles from a multi-scale perspective. We found that the packing structure evolves through a three-step process. Additionally, we developed a quantitative semi-analytical model for the compression curve (Fig. 6). Our findings are broadly applicable to the deformation of HGPs under confining pressure.

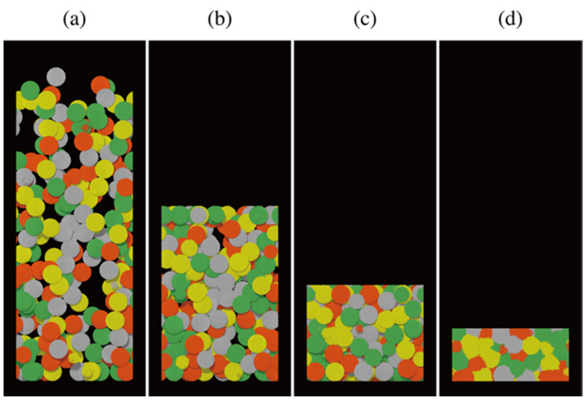

Figure 5: Snapshots of a hierarchical granular pile during compression. The hierarchical granular pile consists of 200 aggregates, and each aggregate consists of 16384 particles. (a) Initial condition. (b) Volume filling factor φ = 16%. (c) φ = 29%. (d) φ = 53%.

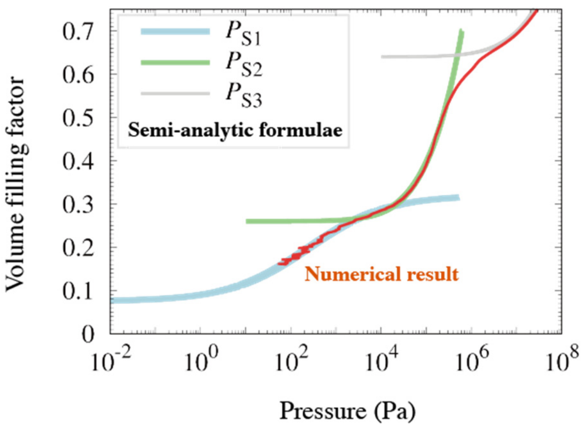

Figure 6: Pressure at the top wall during compression (red) and semi-analytic fittings of the compression curve of hierarchical granular piles (blue, green, gray).

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References

[1] Furuichi, M., Chen. J., Nishiura, D., Arai, and R., Yamamoto, Y., Thrust formation using a numerical granular rock box experiment, *Tectonophysics*, 862, 5, 229963 (2023). 654 DOI:10.1016/j.tecto.2023.229963.

[2] Furuichi, M., Chen. J., Nishiura, D., Arai, and R., Yamamoto, Y., Ide, S., Virtual earthquakes in a numerical granular rock box experiment, Tectonophysics, 874, 11, 230230 (2024). DOI:10.1016/j.tecto.2024.230230

[3] Qin, Y., Chen, J., Singh, S. C., Hananto, N., Carton, H., & Tapponnier, P. "Assessing the risk of potential tsunamigenic earthquakes in the Mentawai region by seismic imaging, Central Sumatra", *Geochemistry, Geophysics, Geosystems*, 25, e2023GC011149, 2024. https:// doi.org/10.1029/2023GC011149.