PhD Final Defense – Seung Jae Lee

Developments in Large Scale Discrete Element Simulations with Polyhedral Particles

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Abstract

Granular material is pervasive in our environment, and of significant importance in a number of science and engineering research fields. It is characterized by the complex behavior, which originates from its discrete nature at the grain scale. Discrete Element Method (DEM) was proposed three decades ago to account for such discontinuity in the materials, and significant algorithmic developments have been made to enhance the performance of DEM. Nevertheless, DEM is still a computationally expensive numerical method to simulate granular materials.

This research focuses on the developments of novel computational methods and tools to conduct large scale discrete element simulations with realistic polyhedral particle modeling, aiming to provide a better insight into the micromechanics of the granular materials. In this dissertation, the research effort is made in two different ways to develop (a) computational methods within the conventional DEM framework, and (b) a new method, impulse-based Discrete Element Method (iDEM). The developed methods are all implemented in a polyhedral DEM code, BLOKS3D, and the performance is quantified to demonstrate the significance of work in terms of computational efficiency and simulation fidelity.

The computational challenges and corresponding developments within the conventional DEM framework are first discussed with the details of modeling approaches to perform two series of polyhedral DEM simulations. The first study envisions the feasibility and viability of using polyhedral DEM approach for lunar regolith simulations, and the second study demonstrates the relative simplicity and reliability to capture the complex triaxial soil behavior with DEM.

A new simulation method, iDEM, is then presented, which significant speed-up of almost two orders for magnitude relative to DEM with reasonable levels of simulation fidelity. This method is formulated on features of the impulse-based dynamic simulation often employed in the computer graphics area where the emphasis is on code speed, numerical stability and physical plausibility. Contact force is not an integral part of the simulation, but required for engineering applications, thus retrieved with a proposed formulation. Therefore, the contact force is a by-product of the simulation that can be retrieved at any time if necessary.