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NUMERICAL SIMULATIONS OF SAND FLOW USING MOLECULAR DYNAMICS APPROACH

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This paper presents a model based on a new type on noncontinuous theoretical mechanical method, molecular dynamics (MD), to simulate the typical soil granular flow. The hertzian friction formula and viscous damping force are introduced in the MD governing equations to model the granular flow. To show the validity of the proposed approach, a benchmark problem of 2D viscous material flow is simulated. The calculated final flow runout distance of the viscous material agrees well with the result of constrained interpolated profile (CIP) method as reported in the literature. Numerical modeling of the propagation of the collapse of three dimensional axisymmetric sand columns is performed by the application of MD models. Comparison of the MD computational runout distance and the obtained distance by experiment shows a high degree of similarity. This indicates that the proposed MD model can accurately represent the evolution of the granular flow. The model developed may thus find applications in various problems involving dense granular flow and large deformations, such as landslides and debris flow. It provides a means for predicting fluidization characteristics of soil large deformation flow disasters and for identification and design of appropriate protective measures.

INTRODUCTION

As a kind of typical granular material, soil causes the common flow forms mainly for earthwork excavation, flow of soils lope by filling, and sudden slip on a weak foundation soil. The large deformation disasters caused by the flow of soil particles have received considerable attention and researches both at home and abroad. At present, the molecular dynamics simulation researches mostly focus on physics, biology, and chemistry, but the application in the field of geotechnical engineering is rare. The molecular dynamics approach is suitable to model granular material and to observe the trajectory of a single particle, so as to possibly identify its dynamical properties. Thus, the molecular dynamics method is tried to be applied to the granular flow characteristics research, and a 3D MD model that simulates granular flow is presented in this work, which is dedicated to provide a strong scientific basis for solving geotechnical engineering problem.

NUMERICAL APPROACH

The accuracy of the model depends on the accuracy of description of external forces acting on the particle and the treatment of collisions. The particles can be either rigid and/or soft. A soft particle model is used in analyzing particle-particle and particle-wall interactions in this paper. The particles are considered to be spherical and identical. The collisions are assumed to be central and involve both linear elastic and damping forces. In the study, 3D ordered granular packings made up of spherical particles are considered. At present, in the field of molecular dynamics, the integral of the motion equation mainly adopts Verlet algorithm. The integral algorithm putted forward by Verlet is the most widely used in the molecular dynamics. The numerical simulations are performed using the molecular dynamics package LAMMPS.

VALIDATION OF THE MD MODEL

The performance of the new model will be verified in this section. It is essential to create an input script containing the

desired commands before running LAMMPS. The Verlet algorithm is applied to the integral of motion equation in the input scripts. When numerical calculation starts, LAMMPS reads the input script, and the displacement, velocity, and acceleration of every granular particle are calculated and updated, thus obtaining the evolution trajectory of the whole calculation system overtime. A two-dimensional simulation of viscous material flow was conducted to verify the reliability of the MD method. Viscous materials flow on the plane under its own gravity, and a literature (Moriguchi, 2005) has detailed calculation and analysis on this flow process using constrained interpolated profile (CIP). CIP method was developed for prediction of large deformations associated with a geomaterial flow, so it can be used as a contrast with the MD method in this work. The model (Wu, 2010) is shown in Figure 1.

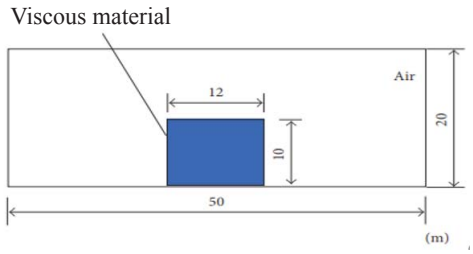

Figure 1. Calculation model (Moriguchi, 2005).

REFERENCES

Moriguchi, S. (2005). *CIP-Based Numerical Analysis for Large Deformation of Geomaterials*. Gifu University, Gifu, Japan.

Wu, B. (2010). Research on preparation and mechanical properties of biomimetic adhesive materials. *Nanjing University of Aeronautics and Astronautics*, Nanjing, China.