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An Investigation of the Extent to which Simulation Can Be Used to Predict the Dynamics of Granular Material

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Abstract

Granular materials, such as sand, gravel, grains, and salt, represent a large portion of the world around us, yet the dynamic behavior of these materials is not well understood. This lack of understanding is due, in large part, to the inherent difficulty in measuring the movement of and forces on individual particles. Computer simulations may be able to provide insight to this problem. Leveraging high-performance computing, simulations can calculate the dynamics (e.g., velocity, acceleration, contact forces) of each particle in a system of granular materials. This tool offers a means to better understand and predict the behavior of granular materials. However, before simulations can be truly useful, they must be shown to be realistic. This effort provides a measure of the accuracy of the simulation software, Chrono::Engine, for two models that investigate slit-flow and piling of granular materials. Data was gathered from physical experiments and then compared to the results of computer simulations. In this way, this research helps to (*i*) determine how closely granular material simulations match reality, and (*ii*) determine avenues for improving granular material simulations.

Contents

1. **Introduction**

The dynamic behavior of granular materials, such as dirt, gravel, grains, salt, and medicine pills, is not well understood. Being able to predict the movement of these materials could benefit a wide range of fields, including studies of tire-terrain interaction, earthquakes, and avalanches; the design of agricultural equipment; and manufacturing methods for such industries as the pharmaceutical industry. The main obstacle to gaining an improved understanding is inherent in the material itself: since it behaves in a massed form, it is somewhat fluidic, but each individual particle of material is a separate body. Thus, granular materials can neither be treated simply as a fluid or solid, and traditional techniques for recording the dynamic behavior of these materials are not easily applicable [11].

Computer simulations may offer a solution to this problem. Leveraging high-performance computing, simulations can calculate the position, velocity, and acceleration of, and forces on each individual particle in a granular material system. However, there are two main challenges with this approach. First, in reality, granular material systems are often very large, with billions or trillions of individual bodies, but this number of bodies is currently very difficult if not impossible to simulate. Other members of the Simulation-Based Engineering Lab are addressing this obstacle by creating and improving algorithms for simulating these large systems [6] [7]. Second, there must be some measure of the simulations' accuracy before they can be fully utilized as a predictive tool. This work aims to address the second challenge.

To provide a measure of the accuracy and predictive abilities of the simulation software, Chrono::Engine [12], this work compares experimental and simulated results for two granular material systems. Similar work was done in 2009 in [4]; the current work repeats and adds to that earlier work to further verify and update the previous results, considering subsequent improvements in Chrono::Engine.

The remainder of this report presents the results from studying two granular material systems. The first system considers the piling of granular materials and is discussed in section 2; the second involves granular material flowing through a slit and is included in section 3.

2. **Piling of Granular Material**

This section considers the accuracy of Chrono::Engine in simulating the piling of granular materials by comparing the angle of repose of the material between experimental and simulated results, and between simulated results and theoretical values. Section 2.1 describes the methods for determining the experimental and simulated results, and a comparison of the two; section 2.2 explains the comparison of the simulations to theory; and section 2.3 presents conclusions on the piling study and areas for future work.

2.1. Comparing Experimental and Simulated Results

In order to provide a measure of the accuracy of piling simulations, the angles of repose from experimental and simulated results were compared.

The angle of repose and static friction coefficient were determined experimentally using glass beads with a diameter of 1 mm. The beads were poured into a glass jar and a picture was taken of the resulting pile (see Figure 1). Using GIMP [3], the angle of repose was measured from the picture as 24.09 degrees. By the equation

$$\mu = \tan\theta \tag{1}$$

where μ is the static friction coefficient and θ is the angle of repose [5], the static friction coefficient was calculated as 0.45.

Figure 1: Experimentally determining the angle of repose of glass beads

A simulation was created with 5,000 spherical bodies, each having a diameter of 1 mm, mass of 1.63E-4 g, and friction equal to the experimentally determined value of 0.45. The simulated results were rendered using POV-Ray [10] and the angle of repose was measured using GIMP as 24.18 degrees (see Figure 2).

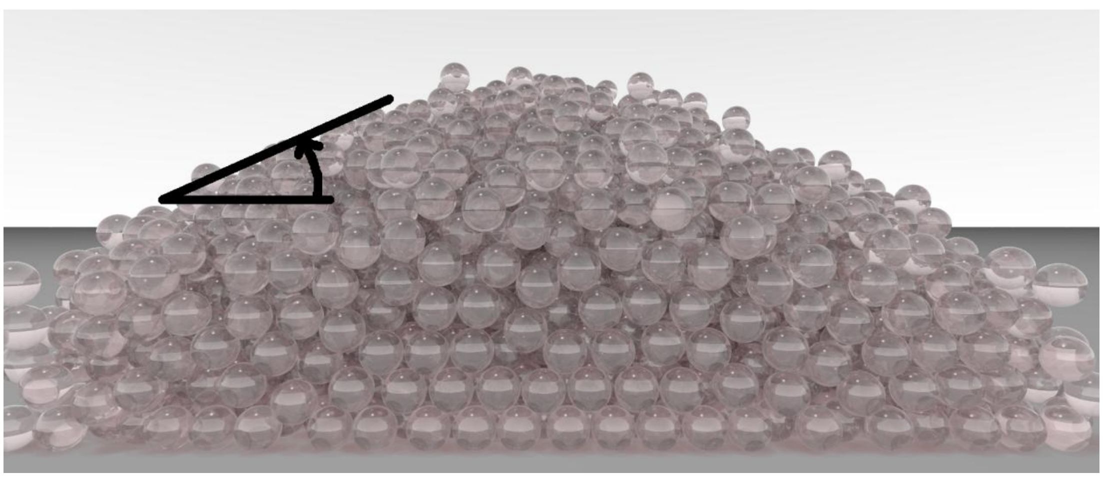

Figure 2: Determining the angle of repose of glass beads by simulation

The experimental and simulated angles of repose are compared in Table 1. The percent error of the simulated angle of repose from the experimental angle, shown in the last row of the table, was calculated to be less than one percent.

Table 1: Comparing experimental and simulated angles of repose

DataSet	Measured Angle (degrees)	Calculated Friction Coefficient
Experiment	24.09	0.45
Simulation	24.18	0.45
% Error:	0.37%	

2.2. Comparing Simulated Results to Theory

In order to more thoroughly test Chrono::Engine's simulation of granular material piling, a number of simulations, each using a different static friction coefficient, were run. Each simulation contains 5,000 spherical bodies, each with a diameter of 1 mm and mass of 1.63E-4 g. The friction values ranged from 0.20 to 1.0.

Once the simulation results were obtained, they were rendered using POV-Ray. Then the angle of repose was measured using GIMP for each simulation (see Figures 3-5). Using these angle values and Equation 1, the static friction coefficients were calculated for each case. Finally, the nominal, assumed friction values were compared to the corresponding calculated friction values. These results, summarized in Table 2, show good agreement between the friction values, with the highest percent error being just over one percent.

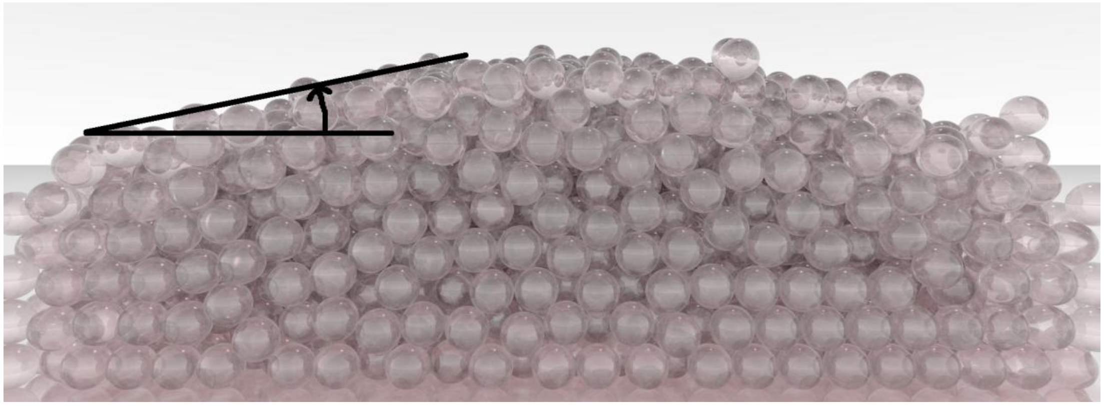

Figure 3: Measuring the angle of repose for the simulation with nominal friction coefficient of 0.20

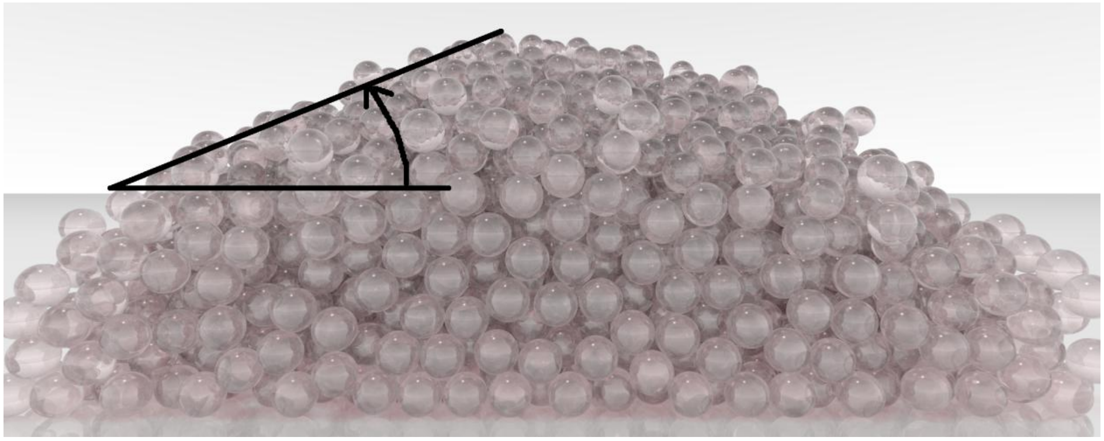

Figure 4: Measuring the angle of repose for the simulation with nominal friction coefficient of 0.40

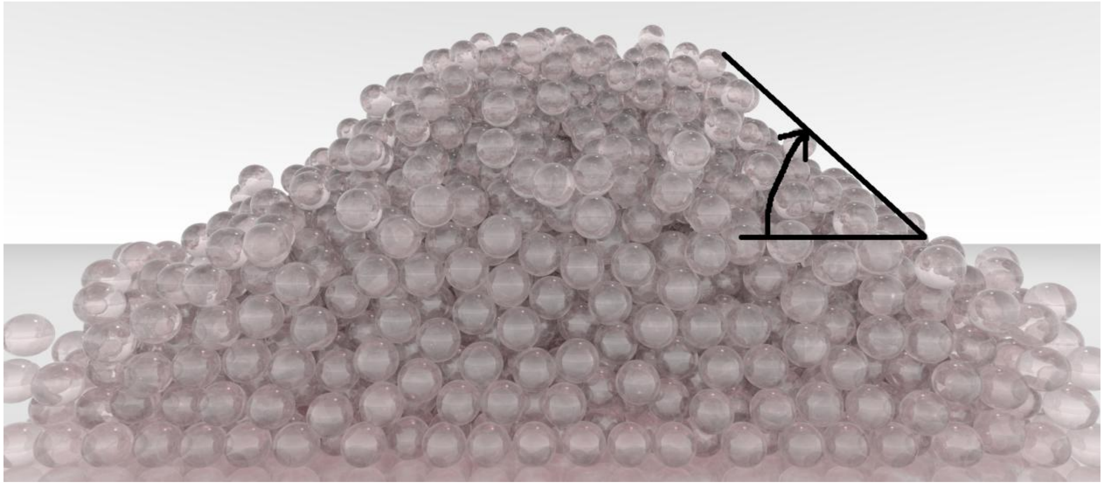

Figure 5: Measuring the angle of repose for the simulation with nominal friction coefficient of 0.90

Table 2: Comparing simulated results to theory

Nominal Friction Coefficient (Assumed in simulation)	Measured Angle (degrees)	Calculated Friction Coefficient (Found using angle)	% Error of Calculated Friction from Nominal Friction
0.20	11.34	0.201	0.27%
0.30	16.68	0.300	0.12%
0.40	21.92	0.402	0.60%
0.50	26.80	0.505	1.03%
0.60	30.83	0.597	0.53%
0.70	34.77	0.694	0.82%
0.80	38.86	0.806	0.72%
0.90	42.16	0.905	0.61%
1.0	44.74	0.991	0.90%

2.3. Piling Conclusions

The results presented in sections 2.1 and 2.2 show very good agreement with the largest percent error between the simulated and experimental results being 1.03%. However, in the simulated case, these results rely on somewhat arbitrary measurement of the angle of repose. While the picture of the actual particles shows a clear edge from which to measure the angle, in the renderings of the simulated particle piles, the edges of the piles are not smooth, leading to difficulty in measuring accurately. To ameliorate the accuracy of this measurement, the simulations could be repeated with a larger number of particles which would result in renders with smoother edges (more similar to what is seen in the actual case), from which the angle of repose could be more easily and accurately measured.

3. Slit Flow of Granular Material

This section considers a model involving granular material flowing through a slit. The model is created both as a physical set-up and as a simulation using Chrono::Engine. Section 3.1 describes the physical and simulated set-ups of the model, while section 3.2 presents a comparison of the results.

3.1. Slit Flow Set-Up Descriptions

For the physical set-up, an aluminum rig, described in [4], was used. A CONEX-controlled LTA_HS high speed motorized actuator [8], connected to a precision double-row ball bearing linear stage [9], controls the opening of the slit. The high-speed actuator was chosen in order to minimize transitional effects due to the opening of the slit. The mass of particles that have flowed through the slit is measured by a LFS 242 tension/compression cell [2]. A force indicator [1] sends the data from the load cell to the computer, where the mass flow rate is then calculated. The system is pictured in Figure 6.

Due to time constraints and technical difficulties with the force indicator, the connection between the computer and load cell was not able to be established for the speed of data recording necessary. In order to confirm the simulated results, data from [4] was used. Future work will include troubleshooting this issue in order to gather new data.

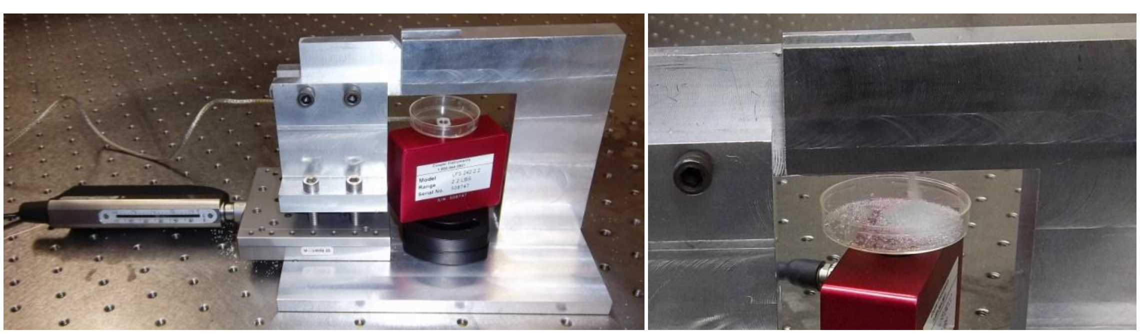

Figure 6: Slit flow model set-up (left), and close-up of material flow (right)

In the simulation, shown in Figure 7, each body is spherical, with a mass of 1.63E-4 g. The slit is opened by applying a motion to the left, sloped body (this motion matches that controlled by the linear actuator in the physical model). The flow rate is calculated by counting the number of bodies below a certain line at each time step, and then multiplying this number by the body mass.

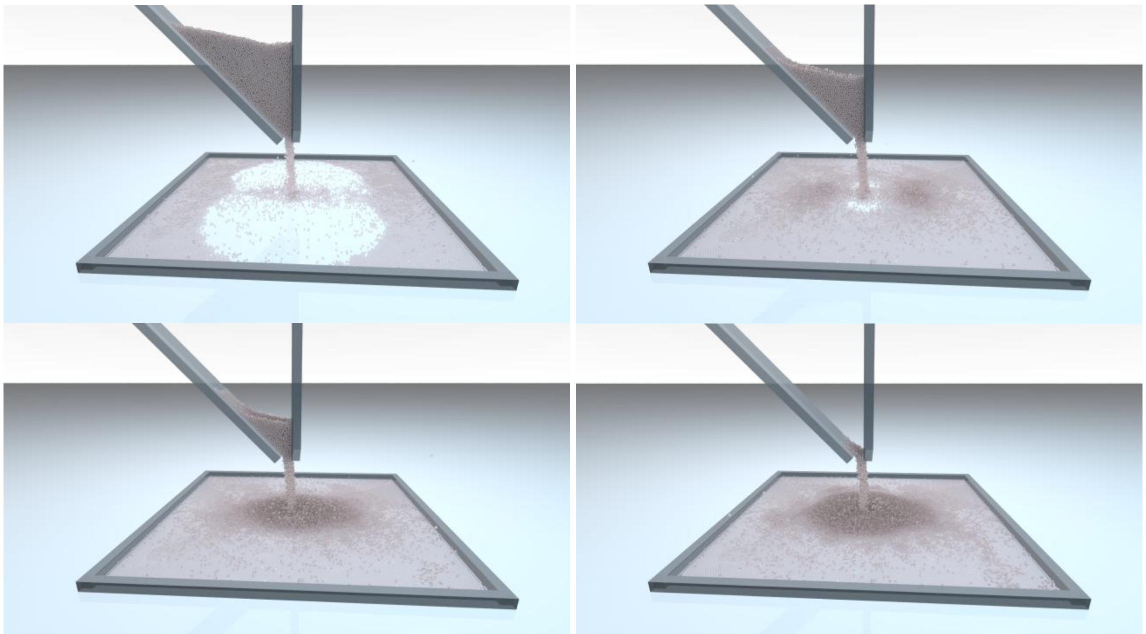

Figure 7: Renderings of four time steps in a simulation of granular material slit flow

3.2. Slit Flow Results

The simulated results are compared to experimental results from [4] in Figure 8. This plot shows five experimental runs (dashed lines), each set up identically, with the only difference being due to the randomness of the granular material flow. The experimental runs are compared to three different simulations; the model is set up the same in each simulation with the only difference being the inter-particle friction coefficient. This friction value is varied between 0.15 and 0.4; the plot shows that the simulation with friction of 0.3 best matches the experimental runs. Assuming all other aspects of the simulation are sufficiently accurate, this shows that the kinetic friction coefficient of the real particles is 0.3.

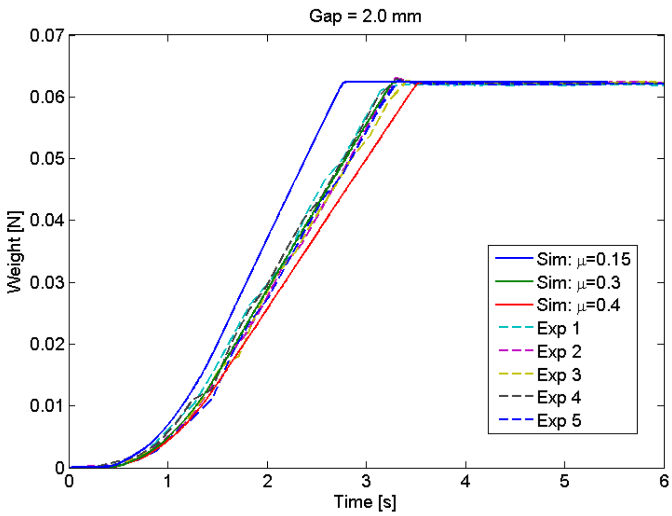

Figure 8: Experimental and simulated mass flow rate data for a gap opening of 2.0 mm

4. Future Work

As mentioned earlier in the report, two shortcomings of this work that require further analysis are (*i*) the difficulty in measuring the angle of repose from the piling simulations and (*ii*) the equipment issues in the physical set-up of the slit-flow model. After addressing these two issues, this work could be expanded on by using different materials with the same models. For example, granular materials of different shapes, such as ellipsoids or seeds; different sizes, i.e., spherical particles that are larger or smaller; and different densities could be studied. Also of interest could be materials that are not uniform. In this way, the effects of these differences could be quantified, while also measuring the accuracy of the simulation software.

5. Acknowledgements

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6. **References**

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