Improving the Precision of Discrete Element Simulations through Calibration Models

Adrian Jensen[1]
Kirk Fraser[2,3]
George Laird[1]
*[1]Predictive Engineering, Portland Oregon*
[2]Predictive Engineering, Quebec Canada
[3]University of Quebec at Chicoutimi

Abstract

The Discrete Element Method (DEM) is fast becoming the numerical method of choice for modelling the flow of granular material. Mining, agriculture and food handling industries, among many others, have been turning their attention towards this powerful analysis technique. In this paper, we present three simple calibration modeling tactics that should be the starting point for every DEM simulation of dry and semi-dry granular material. The three tests are designed to be as simple as possible in order to minimize the run time of the test simulations. The tests are developed to be run in a specific order, providing a sequential calibration procedure that does not involve multiple unknown variables in each test.

Other standard testing methods are briefly discussed, such as the rotating drum and the shear cell (Jenike) tests. The complexity of these tests does not lend itself well to initial numerical model calibration as each test involves many unknown variables. However, they are mentioned as an extension of the three basic test models. The paper will help analysts to increase the precision and validity of their discrete element modelling work.
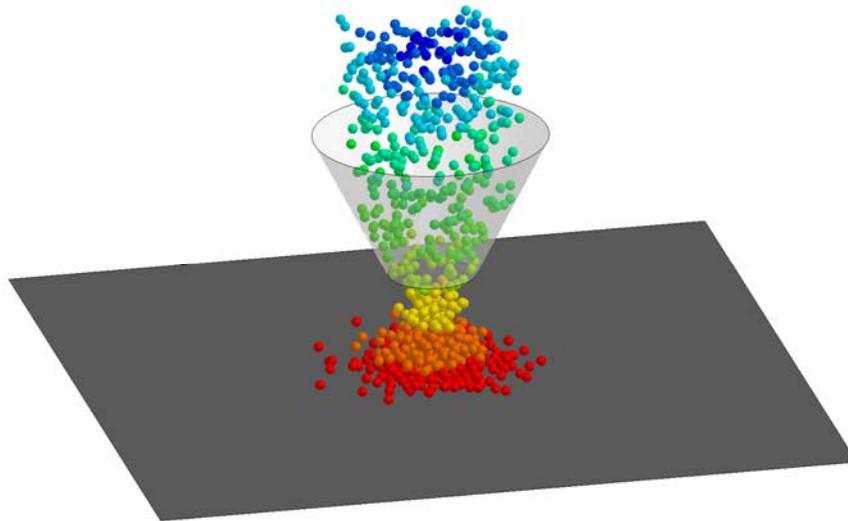
Keywords

Discrete Element Method, Calibration, Granular Material Flow, Improving Simulation Precision, LS-DYNA® Users Conference 2014

Introduction

The objective of this study is to improve the accuracy of Discrete Element Method (DEM) simulations using three simple tests models. Each of the test models is designed to isolate a single physical characteristic of the granular material and allow the analyst to adjust a single model parameter. By focusing the test models in this way, the most accurate model can be generated in the shortest amount of time as the number of parameters to adjust is minimized.

Granular material can be difficult to idealize because although the individual particles are solid, the bulk material behaves more like a fluid. The shear stress that a bulk material can withstand is much less that the shear strength of a single particle of the same material. Furthermore, the shear strength of the bulk material may be more dependent on particle size and shape than the shear strength of the particle material. Common examples of granular material include coffee, sand, grains, wood chips, pepper, soil, beans, ball bearings, and gravel.

The discrete element method is a powerful tool that can be used to model many different types of granular flow problems. Material flow from one conveyor to another through a transfer point is a common application for DEM. Hastie and Wypnch [1] use DEM to model such flows and compare it to continuum based approaches. In recent years, coupling DEM with other numerical methods such as CFD and heat transfer has become possible. Bluhm-Drenhaus *et al*. [2] use a coupled DEM-CFD approach for investigation of the conversion of limestone to quicklime. Grima and Wypnch [3] outline an elaborate calibration approach, but their method requires extensive equipment setup. Coetzee and Els [4] provide a comprehensive calibration method for two dimensional DEM simulations. The purpose of our work is to provide simple calibration tests that can be run quickly without the need for significant equipment setup.

The methods described in this paper were designed for dry granular material. The three tests outlined here are a good starting point when working with moist materials, but more calibration tests are necessary to fully capture the capillary forces that exist between wet particles. Wet material can be modeled in LS-DYNA® with DEM by setting `CAP=1` on `*CONTROL_DISCRETE_ELEMENT`. The parameters that define the behavior of wet material can be found from the equations developed by Rabinovich *et al*. [5, 6]. Another key assumption is that the material is more likely to slide than it is to roll. That is, the application of these methods assumes the end goal of the analysis is to capture the bulk flow of granular materials, not the behavior of a single layer of particles.

Background

The Discrete Element Method referenced in this paper was first developed by Cundall *et al*. in 1971 [7] for rock and soil applications. The basic concept is that a granular material can be idealized with small rigid spheres (some codes allow modeling of arbitrary shapes) and the interaction of these spheres captures the behavior of the bulk material. Each sphere obeys Newton's laws and the laws of particle motion. The interaction of spheres with each other and with boundary surfaces is handled by contact algorithms.
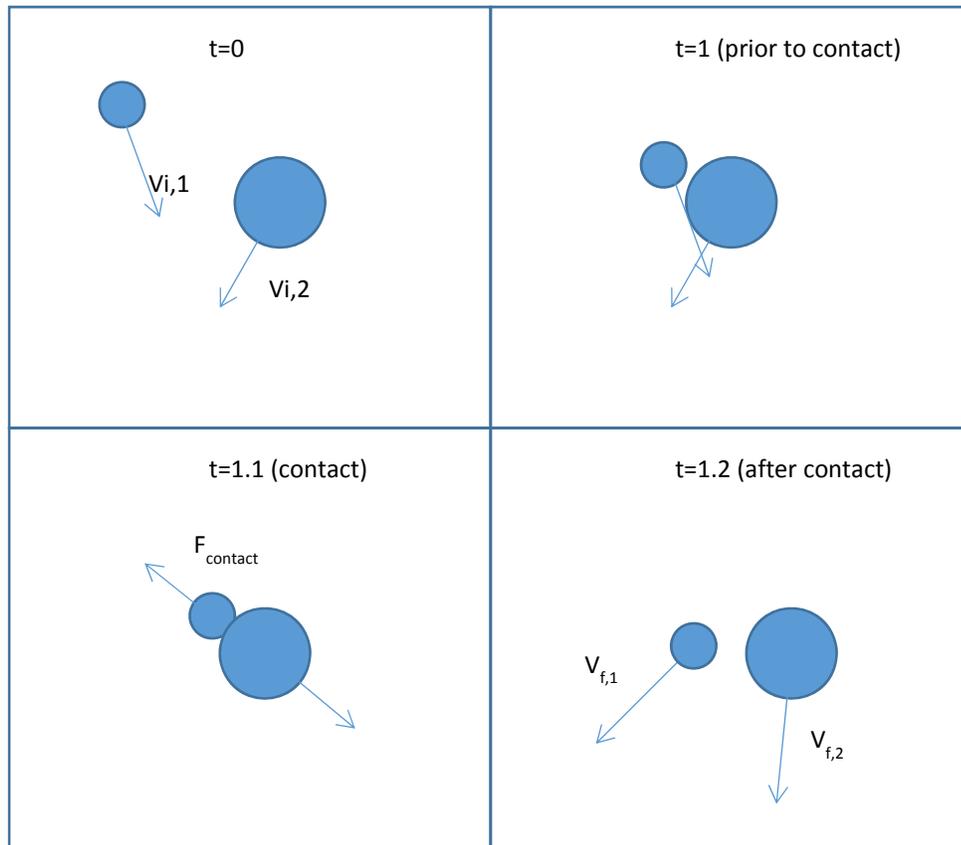
Motion (position, *s* and velocity, *v*) of particles is calculated in space for each time step:

$$v = v_i + a(\delta t)$$

$$s = s_i + v_i(\delta t) + \frac{1}{2}a(\delta t)^2$$

At impact, a contact force is calculated proportional to the stiffness of the particles, position and velocity. Momentum before and after impact is conserved:

$$M_1 v_{i1} + M_2 v_{i2} = e(M_1 v_{f1} + M_2 v_{f2})$$

Where "*e*" is the coefficient of restitution (this depends on many factors: friction, cohesion, adhesion, etc.). The time steps must be small enough to ensure that there is no penetration of the particles, otherwise the force applied to separate the spheres will be too large and the system will become unstable (exploding nodes).

The computational cost of a typical DEM simulation is very high; models can take days or weeks to run for a meaningful number of particles (in the multi-million range). A lot of work has been done recently to parallelize the DEM method using graphics cards. There are a number of research groups working on accelerating DEM. For example, Govender et al. [8] have used CUDA C/C++ to write a polyhedron DEM solver that is very fast and efficient.

Time Step

As all of the models in the paper are analyzed with the explicit solver, it is necessary to calculate a time step. In order to ensure stability of the numerical method, a minimum time step can be determined based on the Raleigh, Hertz or Cundall approach. In this project, twenty percent (0.20) of the Cundall time step is used to set the simulation time step. The Raleigh and Hertz time step sizes are described in LIGGGHTS documentation [9]:

Raleigh time step:

$$dt_{raleigh} = \frac{\pi \, r_{sphere}}{0.1631(v + 0.8766)} \sqrt{\frac{\rho}{E/[2(1 + v)]}}$$

Where r_{sphere} is the radius of the smallest particle in the model, ρ is the particle density, E is the modulus of elasticity and v is poisons ratio.

Hertz time step:

$$dt_{hertz} = 2.87 \left[\frac{(\rho(4/3) \, \pi \, r_{shere}{}^3)^2}{r_{sphere} \, E^2 \, V_{max}} \right]^{0.2}$$

Where V_{max} is the maximum relative velocity expected during the simulation (taking into account any mesh motion).

Cundall time step is used in the LS-DYNA DEM code [10]:

$$dt_{cundall} = 0.2 \, \pi \sqrt{\frac{\rho(4/3) \, \pi \, r_{sphere}{}^2}{\frac{E}{[3(1 + 2v)]} \, NORMK}}$$

NORMK is a stiffness penalty parameter; it is typically taken as 0.1 to 0.001.

Stability of the numerical method can be ensured by setting the time step equal to 20% of the minimum of the previously mentioned methods.

$$dt = 0.2 \, \min(dt_{raleigh}, dt_{hertz}, dt_{cundall})$$

DEM Particle Size

When choosing discrete element particle size, an analyst has many variables to consider. The first consideration is the overall element count. The capability to solve complex DEM simulations on a personal computer is relatively new and is limited by the overall element count to keep the computation times reasonable. When working with the test procedures described in this paper, minimizing the solution time is critical because the model will be analyzed many times in order to converge on accurate parameter values.

The ideal analysis scenario is when the actual particle count is a reasonable number of elements to analyze for a given computer system. In this scenario, actual particle size can be used for the discrete elements. More commonly, the actual particle size is much smaller and number of individual particles is much greater. Therefore, using actual particle size is computational prohibitive. When this is the case, choosing DEM particle size is analogous to meshing with Finite Elements; enough elements must be used such that accurate behavior of the system is captured but not so many elements that the analysis cannot be run in a reasonable amount of time.

To capture the bulk flow of the material, it is suggested that at least 8 elements fit across the width of any bulk material handling device. That is, the diameter of the DEM particle should be no greater than $1/8^{th}$ the width of a hopper, conveyer belt, screw conveyor, bucket or other container. When the granular material is flowing through an opening, the same rule-of-thumb applies: the maximum diameter of the DEM particle should be $1/8^{th}$ the diameter of the opening. When the granular material is assembled into a conical pile, e.g., via a stacker, the pile height will need to exceed 15x the DEM particle diameter to accurately capture material behavior.

These general sizing guidelines can be viewed in two ways: if the DEM particle size is held constant, the geometry of the simulation (hopper width, pile height, etc.) must be scaled to meet the demand. If the geometry of the bulk material handling equipment is provided, the DEM particle size must be adjusted. The first approach is used for the tests performed and documented in this paper.

Generating DEM Particles

For the tests described in this paper, the DEM particles are generated using `*DEFINE_DE_INJECTION`. This method allows the user to define a plane where the discrete elements will be created with given mass flow rate, minimum size and maximum size. Alternatively, LS-PrePost® can generate a set of discrete elements using the sphere packing engine. This requires the user to provide an enclosed volume meshed with shell elements. The spherical elements generated within this volume will use a constant user-defined radius [11].

Calibration Test Procedures

The concept of the calibration tests is simple; given three granular material properties (bulk density, angle to induce flow, poured angle of repose), three test models (volume test, surface friction test, internal friction test) performed in sequential order will allow the analyst to adjust three model parameters (`*MAT_ELASTIC RO`, `*DEFINE_DE_TO_SURFACE_COUPLING FricS/FricD`, `*CONTROL_DISCRETE_ELEMENT Fric/FricR`) resulting in an accurate idealization of the granular material. The sequence of these tests is such that for a given test, the specific parameter to be calibrated does not have a dominant effect in the previous test(s). For example, for the final test (Internal Friction Test – Poured Angle of Repose) both bulk density and surface friction may have a significant effect on the results but the internal friction, the parameter of interest for this test, does not weigh heavily on the prior tests.

Volume Test – Bulk Density

The first of the three tests is the volume test. Given a bulk density, this test allows the analyst to adjust the particle density (material density used for the DEM particles). Often, the actual density

of an individual particle is not known, only the bulk density. However, The DEM software requires the analyst to provide a particle density and not a bulk density.

This simulation requires a container to hold the DEM particles, a scraper to level the DEM particles with the top of the container and of course, the DEM particles.
This test consists of three distinct stages:
- Injection – during this stage, the DEM particles are generated and fill the container
- Settling – this stage allows time for the DEM particles to reach static equilibrium
- Scraping – the scraper moves across the top of the container and removes excess particles

During injection and settling, the container is being vibrated to assist in the packing of element into the container. A summary of the simulation steps are listed in the table below.

Simulation Step	Start Time (sec)	End Time (sec)	Duration (sec)
Injection	0.0	2.0	2.0
Settling	2.0	3.0	1.0
Vibration	0.0	2.5	2.5
Scraping	3.0	10.0	7.0

Once the scraper has removed all excess material from the container, the mass of the elements within the container is recovered from the model. Dividing the total mass of the elements within the container by the volume of the container yields the bulk density. Adjusting the bulk density is a simple process where the initial particle density (RO on the *MAT_ELASTIC card) is scaled by the ratio of the bulk density calculated from the simulation to the given bulk density of the actual granular material. Unlike the other tests, this is not an iterative process and once the material density is adjusted, the bulk density will match the data.

The series of figures below illustrates the injection and settling stages of the process. The first image shows the model as the DEM injection fist starts. The next image show the container overflowing as the elements settle into place. The final image shows the container with the elements in static equilibrium and ready for the scraping stage of the process.
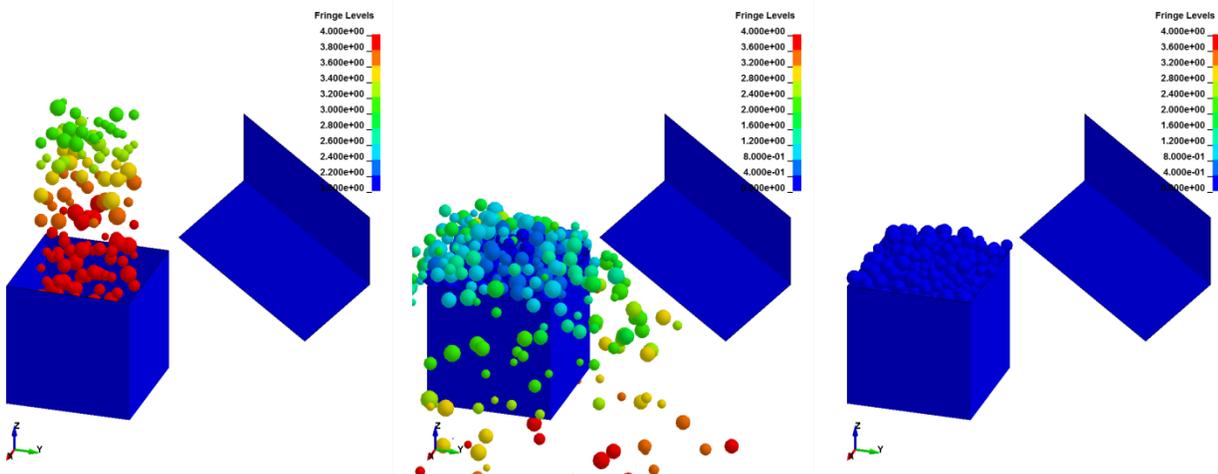
The next series of images shows the scraping process. The scraper moves across the top of the container leveling off any excess material.
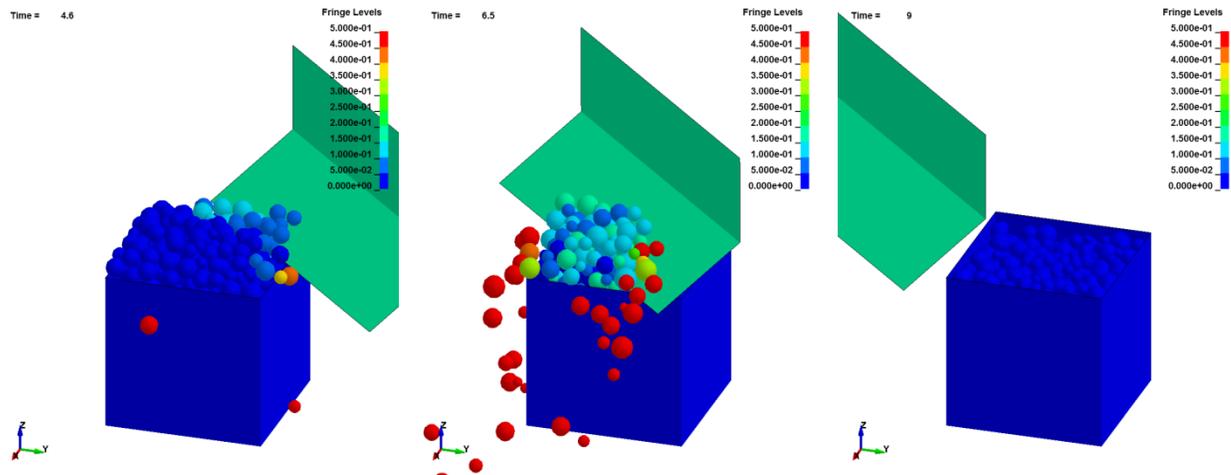
### Surface Friction Test – Angle to Induce Flow

The next test is the surface friction test. At this stage of the calibration process, the particle size, distribution and density has been set. As mentioned in the Background section, when the DEM particle size is set, the geometry of the test fixture may need to be adjusted to accommodate the element sizing guidelines.

The goal of this test is to calibrate the coefficient of friction between the DEM particles and the surfaces that they will come in contact with. If the DEM simulation will have the DEM particles in contact with multiple materials, this test should be performed for each material. This test consists of a long narrow chute with side walls. When the analysis first starts, a temporary wall (the gate) is in place to keep the DEM particles clustered at one end of the chute. Once all DEM particles have settled in the starting area, the gate is lifted. The chute slowly rotates until the angle of the chute is steep enough that the DEM particles start to slide.
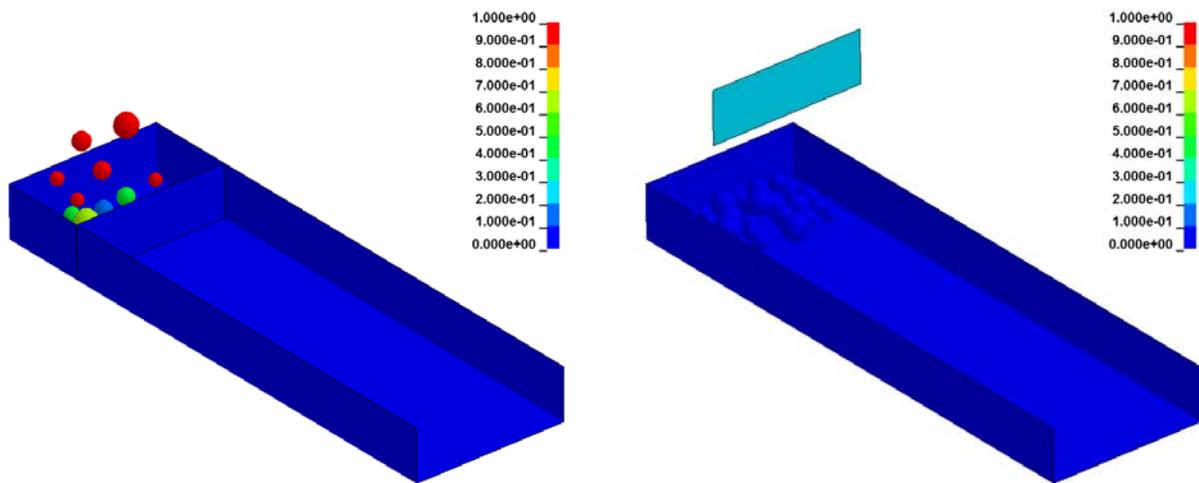
This test consists of five distinct stages:

- Injection – during this stage, the DEM particles are generated and fill the container.
- Settling – this stage allows time for the DEM particles to reach static equilibrium
- Gate Movement – the gate is lifted and henceforth plays no role in the simulation
- Settling – a second settling stage allows the particles to relax in the absence of the gate
- Surface Tipping – the chute is rotated until the particles start to slide
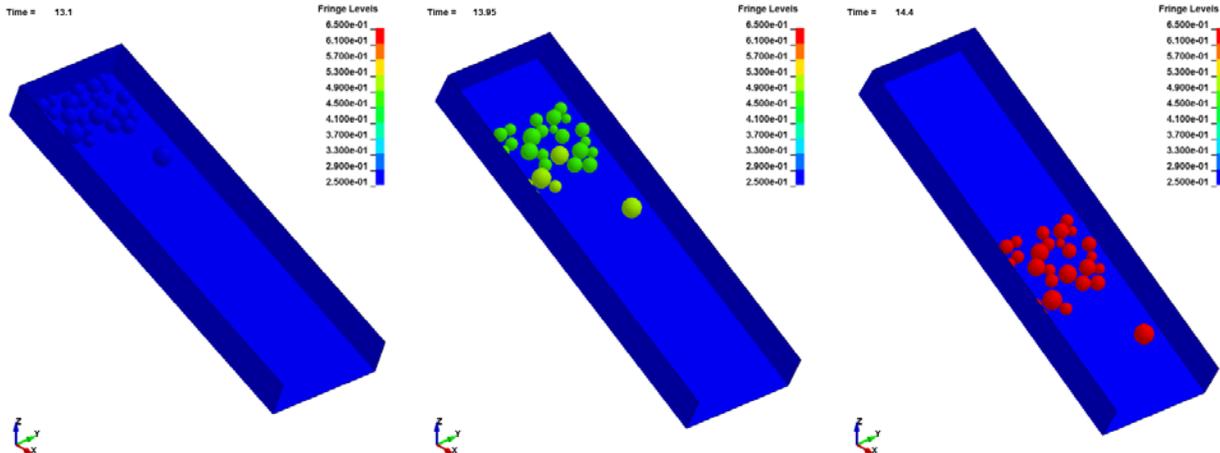
As with the previous simulation, a subtle vibration is applied to the container using `*BOUNDARY_PRESCRIBED_MOTION_RIGID` with a sine function and a magnitude of 0.002 m. In the case of this test, the goal is not to encourage the packing of elements but rather minimize the energy state of the bulk material. If the elements are packed into the staging area too tightly, it is possible they will move significantly once the gate is lifted and thus make it difficult to determine the true chute angle that instigates sliding. A summary of the simulation steps are listed in the table below.

Simulation Step	Start Time (sec)	End Time (sec)	Duration (sec)
Injection	0.0	1.0	1.0
Settling	1.0	3.0	2.0
Vibration	0.0	2.0	2.0
Gate Movement	3.0	5.0	2.0
Settling	3.0	10.0	7.0
Surface tipping	10.0	20.0	10.0

Extracting results from this model is incredibly simple. Once the pile of material starts to slide, the simulation is stopped and the angle of the chute is measured. The key is to recognize the initial movement of the bulk material and ignore any outliers such as a single element that is rolling across the surface before tipping begins. Unlike the first test, the relationship between the measured output and the parameter to be calibrated is not linear. That is, finding an accurate coefficient of friction between the DEM particles and the surface is an iterative process. An initial value must be guessed and subsequent guesses must be guided by the discrepancy between the angle to induce sliding in the simulation and the true angle to induce sliding.

This iterative process is outlined below:
- Choose a guess value for the coefficient of friction
- Run the simulation
- Determine the critical chute angle for material motion
- Calculate a gradient between the obtained chute angle and the desired critical angle
- Use the gradient to determine a new guess value for the friction coefficient
- Iterate steps 2 to 5 until a reasonable tolerance is obtained

The friction value(s) that are being changed during this process are found within the
`*DEFINE_DE_TO_SURFACE_COUPLING` card. `FricS` and `FricD` are the parameters to be
adjusted with each iteration. As stated in the Background section, the goal of these simulations is
to capture the bulk flow of granular materials. Therefore, the difference between sliding friction
(`FricS`) and rolling friction (`FricD`) is negligible in this application and the same value will be
used for both. The iteration process converges fairly quickly with this procedure (typically 3 to 4
iterations).

**Internal Friction Test – Poured Angle of Repose**
The third and final test in the series will help calibrate the internal friction or friction between
discrete elements. When the analysis first starts, a cone is stationed over a flat horizontal plate.
DEM particles are generated above the cone and as they fall through the opening, they form a
conical pile. At a certain point the top of the conical pile will reach the opening at the bottom of
the cone. The cone is moved upward and the pile is allowed to grow uninhibited.
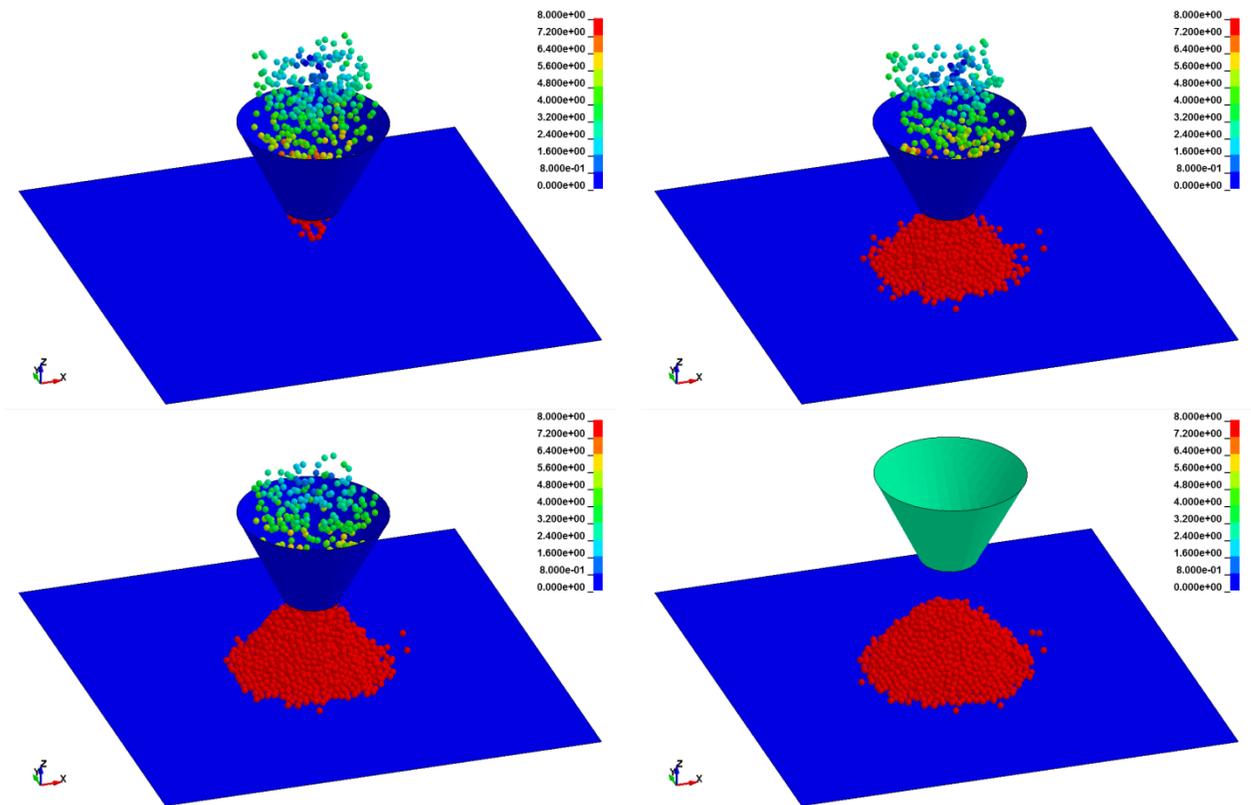
A summary of the simulation steps are listed in the table below.

Simulation Step	Start Time (sec)	End Time (sec)	Duration (sec)
Injection	0.0	7.0	7.0
Cone Movement	5.0	15.0	10.0
Settling	7.0	18.0	11.0

Once the settling is complete, the angle of the conical pile with respect to the flat surface is measured. This is called the angle of repose. As with the previous test, the dimensions of the test fixture may need to be adjusted to accommodate the DEM particle size. In this case, the analyst must consider the geometry of the fixture and the overall volume of the particles being used. If too few particles are used to generate the pile, the angle of repose will be inaccurate or difficult to measure. Although guidelines are provided, visual inspection of the simulation results is sufficient to determine if enough elements are used.
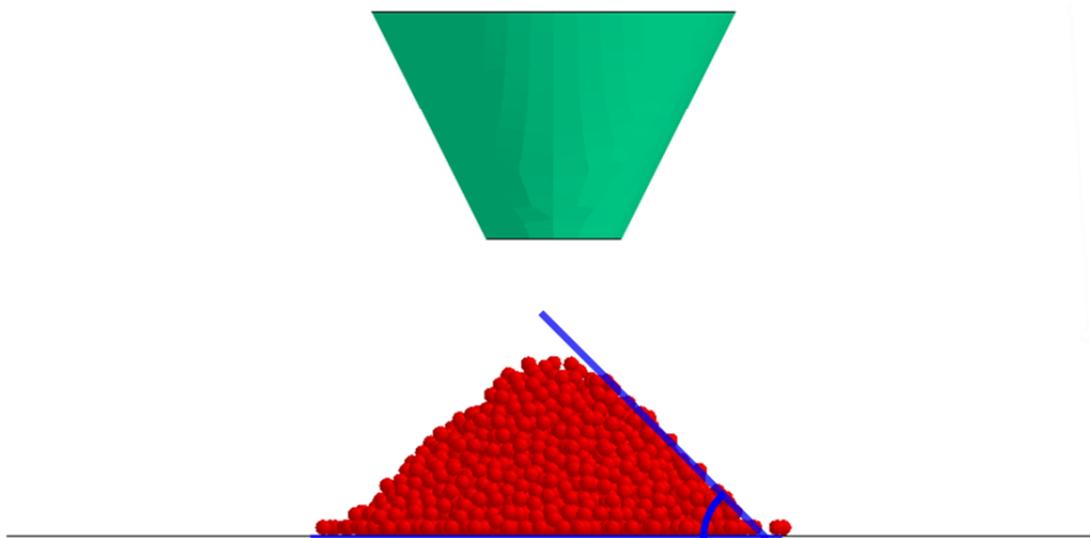

Like the Surface Friction Test, this test is an iterative process:
- Choose a guess value for the coefficient of friction
- Run the simulation
- Determine the angle of repose
- Calculate a gradient between the obtained angle or repose and the desired angle of repose
- Use the gradient to determine a new guess value for the friction coefficient
- Iterate steps 2 to 5 until a reasonable tolerance is obtained

The friction value(s) that are being changed during this process are found within the `*CONTROL_DISCRETE_ELEMENT` card. `Fric` and `FricR` are the parameters to be adjusted with each iteration; the same value should be used for both parameters.

Additional Test Procedures

While the intent of this paper is to propose three simple tests to help improve accuracy of discrete element simulations, it should be noted that other calibration tests exist.
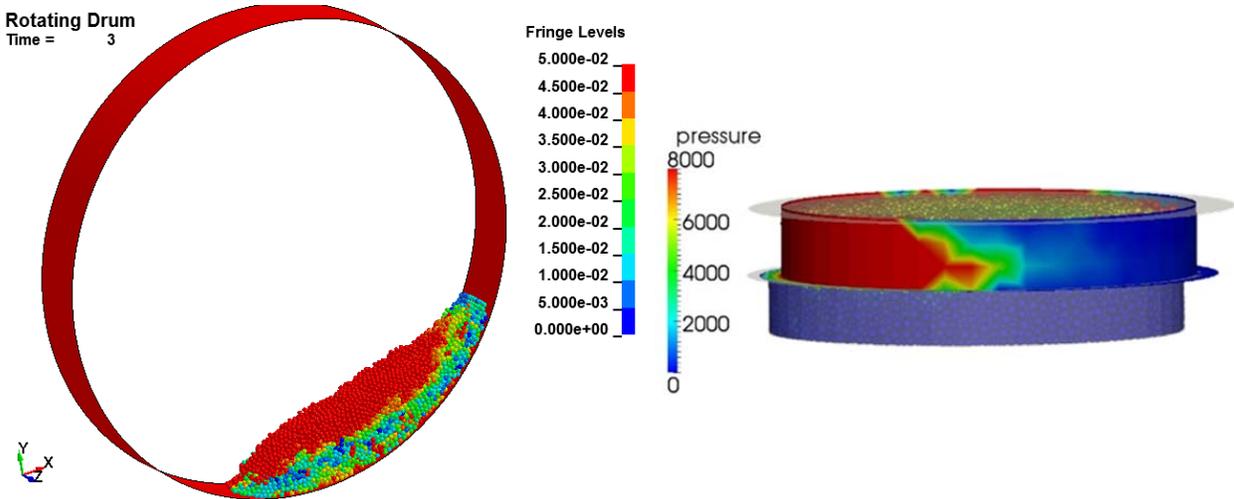
Rotating Drum

Typically, the angle of repose of a vibrating, rotating or moving granular sample will be different than that of a static sample. This test is designed to calibrate the angle of repose of a moving bulk flow. An example of the rotating drum test is shown above on the left-hand side.

Jenike Shear Cell

This test can be used to determine many different parameters of a bulk material such as internal friction, wall friction, etc. The primary purpose of the test is to determine the shear strength of the material. A large number of parameters need to be "dialed in" when trying to calibrate a model. As such, calibration with this method should only be attempted if the three basic tests have been performed. An example of a Jenike shear cell test is shown above on the right-hand side. The test is difficult to reproduce numerically because a force or displacement control is needed on the cover of the shear cell. More information on this test is available in reference [12].

Conclusions

The objective of these calibration models is to improve the precision of DEM simulations. The test models should be compact and efficient allowing for many iterations with quick computing times. We use these calibration models as a starting point for all the DEM consulting work that we do. As with all simulations, exactness is lost in idealization. The accuracy of the input parameters used for a DEM simulation can be improved with these simple calibration models.

Acknowledgements

LS-DYNA Input Decks
For any interested parties, please contact the authors for access to the input decks.

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