Simulating Granular Dynamics using High Throughput Computing

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The research that I would use high throughput computing for pertains to the field of granular dynamics. Granular materials are quite ubiquitous; they are the sugar you put in your coffee, asphalt on your driveway, salt, powder used to make antibiotics, pills, as well as meteorites and avalanches. The researchers in this field seek to understand how granular materials behave when they are subjected to continuous vibrations, taps, and shearing. This research can be traced back to the 1600s with regard to studies that Johannes Kepler did to understand the geometry of snowflakes. One important problem that is studied with regard to granular materials is how well they "pack." The packing problem that I am interested in deals with tuning vibration parameters (amplitude and frequency) that will make a system of particles achieve a highly organized as well as densely packed states.

The problem of the packing of granular materials I have studied involved modeling a system of granular particles as idealized monodispersed spheres (see Figure 1) in a parallelepiped vessel using both stochastic and deterministic methods.

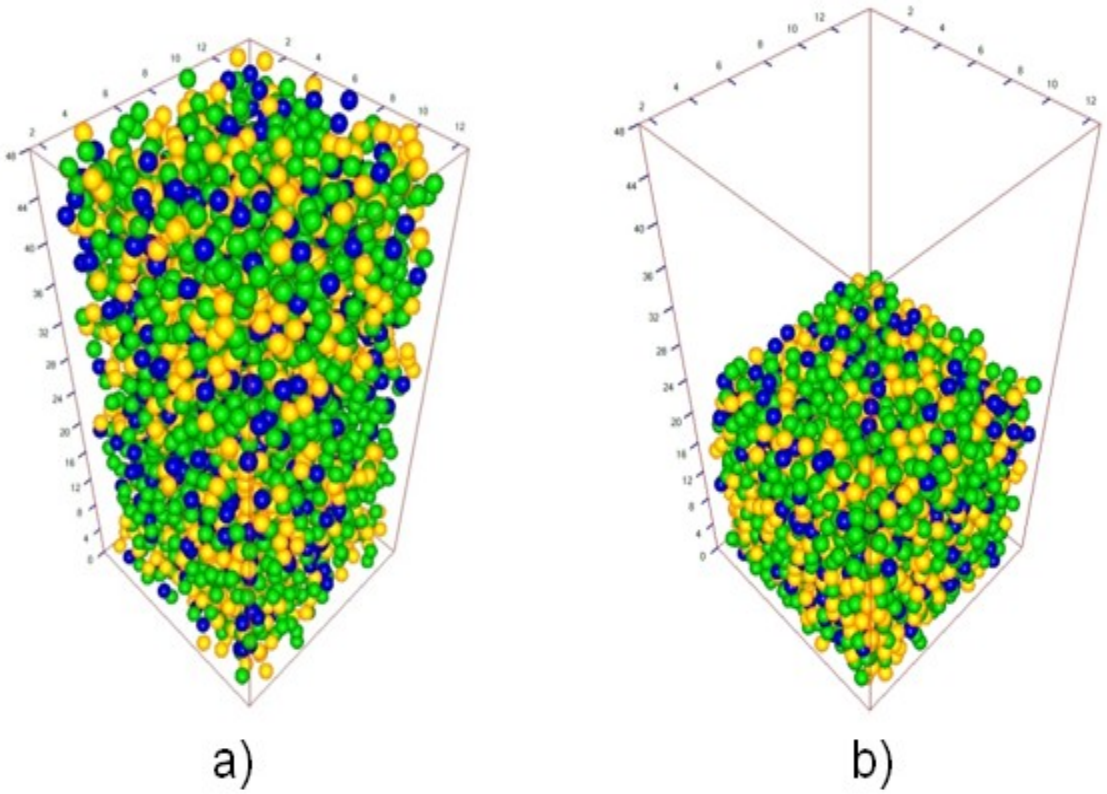


Figure 1: a) Representation of a system of particles in an expanded state (the vessel was tapped). b) Representation of a system of particles after they have settled to a quiescent state.

For the stochastic method, a Monte Carlo simulation was used. In the MC simulation, a single step in the algorithm (MC step) consists of the random selection of a particle, followed by its assignment to a trial position. The trial position is accepted unconditionally (provided that an overlap does not occur) as the new location if the change in the system energy is less than or equal to zero. Otherwise, if the change in energy is positive, the trial position is accepted with a certain probability. Another particle is then selected at random, and the above procedure is repeated. The effect of a single tap applied to a containment vessel filled with spherical particles of diameter d is idealized by lifting the entire particle assembly from the floor by an amount Δ, whose normalized value is $\gamma \equiv \Delta / d$ as shown in Figure 2 below.

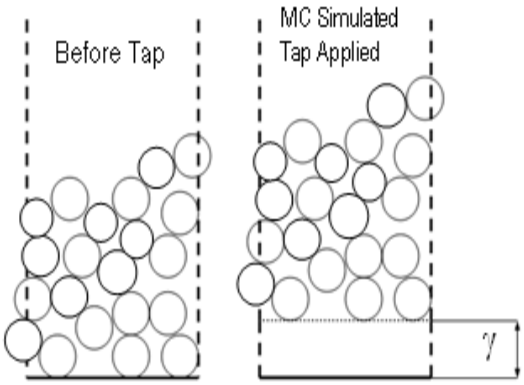


Figure 2: Tapping protocol for the MC simulation.

The key quantity that is to be calculated is the bulk solids fraction (the ratio of solids occupied to total volume of the vessel). For our simulations (both deterministic and stochastic) we usually plot the solids fraction as a function of time to determine how the density of the system evolves. The solids fraction is measured every 10^6 MC steps, and the settling process stops when the difference in solids fraction between every 10^6 k MC steps is less than a certain tolerance. For the Monte Carlo simulations, we have 100 ensembles of particle systems, and we then calculate the ensemble averaged evolution of the solids fraction.

The deterministic method that was used is called the discrete element method (DEM). In that method, Newton's equations of motions are solved for the system of particles. One can think of the DEM as just dissipative molecular dynamics. The tapping protocol used in the DEM simulations is a half-sine wave that is applied to the base of the vessel. After the tap is applied, a period of relaxation is then followed so that the system is quiescent. The solids fraction is then measured after the period of relaxation. This tapping followed by a period of relaxation is repeatedly applied until the density of the system equilibrates to some value. Just like the MC simulation, we also look at the ensemble averaged solids fraction evolution. Therefore we run approximately 20-25 ensembles for a specific vibration case. An example of an ensemble averaged solids fraction evolution plot is shown below in Figure 3 for two different cases.

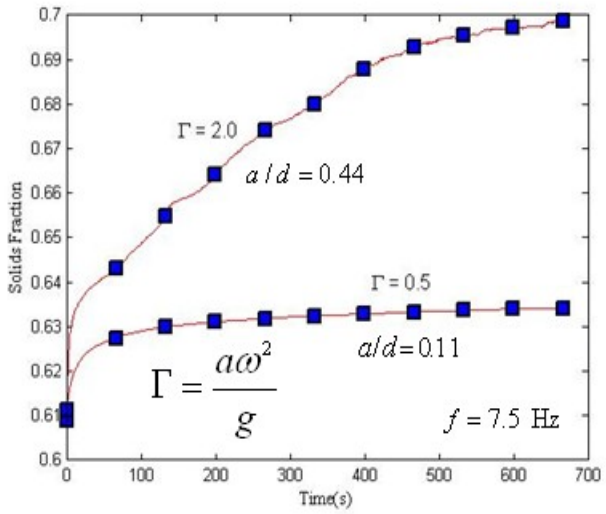
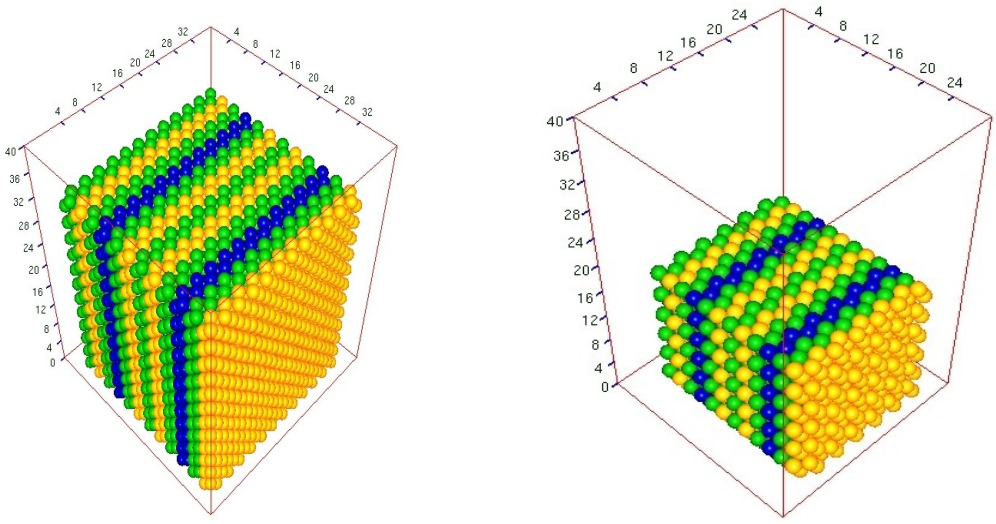


Figure 3: Solids fraction evolution as a function of time for DEM simulations of two sets of vibration parameters (frequency of 7.5 Hertz and two different amplitudes to particle diameter ratios *a/d).*

One case is where they system of particles attain a large solids fraction (~0.697) while the other case had a smaller solids fraction (~0.63). Just for comparison, the maximum solids fraction for a system of spheres is approximately 0.74 which is measured in a face-centered-cubic crystal (FCC) or hexagonal-closed pack crystal (HCP) (see Figure 4). Therefore the case in Figure 3 above that has a solids fraction of 0.697 is quite densely packed when compared to FCC and HCP structures.



a) b)

Figure 4: a) Face Centered Cubic Crystal b) Hexagonal Closed Pack Crystal

The use of grid computing to run both the Monte Carlo and DEM simulations is one that I have taken advantage of. For both types of simulations, it is more advantageous to use HTC rather than HPC because my research group and I are interested in investigating different cases concerning the vibration parameters, i.e. the frequency and amplitude of a tap, so we are more concerned with the amount of processors to run our jobs rather than how fast our jobs finish. We have made use of OSG resources with the help of Mats Rynge to run both our Monte Carlo and DEM simulations. We were able to complete substantial amounts of case studies and analyze the data which yielded quite interesting results. One important result that was obtained was that for the MC simulations the final packing of the system of particles was independent of the initial state. We will also run DEM simulations to confirm the aforementioned observation.

The amount of data that we output does vary depending on the type of simulation. For example, in the MC simulations, there would be about 4 output files, where the maximum amount of data would be less than a megabyte per simulation run. However, we would have about 600 runs, so then the total output would be around 600 megabytes. For the DEM case studies, we would have about four to five files; however, for one run the amount of data would be around 40 megabytes. We would then have about 2000 runs, so there would be a substantial amount of data that would be generated. The data would be stored on my OSG account or the scratch space; however, I would transfer the files to my local directory at my school to post-process the data.

For the MC simulations, the run time for a particular ensemble is approximately 1 day. In that one day, about 1000 taps are completed for each realization. While for the DEM, the run time is also a day; however, the amount of taps performed are about 20-160 taps depending on the amount of particles in the vessel. The reason that the run time was chosen for a day is so that most of the jobs can finish running successfully when submitted to the OSG resources. The script files that are being used make use of OSG Match Maker to submit the jobs to various resources. An important parameter in the submit script is the parameter that specifies the maximum amount of wall clock time for each simulation as well as the amount of memory for each job as those parameters will determine the rank of the resources which will be best suited to run our jobs.

Without OSG, the previous MC case studies as well as the DEM case studies that I will be running would not be possible to investigate as we do not have that amount of resources available in our research group. Thus, the resources provided by OSG will continue to allow us to get more done in our research.

References

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