Project Report on Granular Media

A project report submitted

by

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Introduction:

Granular media consist of collections of discrete particles or grains that exhibit unique mechanical and physical behaviors not commonly found in conventional solids, liquids, or gases. These particles interact through contact forces, which include frictional and collisional interactions. The collective behavior of granular materials under various external stimuli, such as compression and shearing, often displays non-linear and emergent properties, making them an important subject of study in fields such as physics, material science, and engineering.

This project focuses on the simulation of a 2D granular system enclosed in a square box. The system is composed of 2 different types of particles, which are subjected to repeated cycles of unidirectional compression and decompression from the top and bottom gran walls. The primary objective is to analyze how the pressure exerted on the system evolves as the packing fraction changes during these cycles. The packing fraction, defined as the ratio of the area occupied by particles to the total area of the container, serves as a key parameter influencing the behavior of granular media.

By simulating these compression and decompression cycles, valuable insights can be gained into the pressure response and the mechanical properties of granular materials under varying density conditions. The project utilizes LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) for modeling and data generation, with a focus on extracting and analyzing pressure as a function of packing fraction to understand the system's behavior during different stages of compaction and relaxation.

Methodology:

This section details the process and techniques used in simulating a 2D granular system in LAMMPS to study the relationship between pressure and packing fraction.

1. Simulation Setup in LAMMPS:

Container Design: The simulation box was set up as a 2D structure with walls composed of smaller granular particles to act as boundaries for the main particle system. The top and bottom wall particles are used to compress and decompress the system.

Particle Initialization: Two different types of particles were defined of diameter 0.5 and 0.7 and inserted into the box to create a heterogeneous granular medium. The initial arrangement of particles was configured to achieve a packing fraction of 0.3, representing a loosely packed system.

2. Simulation Parameters and Commands:

Initial Pair Style for Particle Generation:

A square simulation box of side 50m is formed. Initially to create the particle lattice with a packing fraction of 0.3, the **pair_style soft command** was used in the region 43×43. This allowed the particles to be placed without significant overlaps and provided a stable starting configuration.

Contact Mechanics:

During the main simulation, the **pair_style gran/hertz/history** was employed for all active particles. This pair style models particle interactions based on Hertzian contact mechanics, incorporating both normal force and tangential frictional history to accurately represent real granular behavior.

Wall Movement:

The **fix move command** was applied to the wall particles to control their compression and decompression. The compression speed was set to a low value of **0.005 m/s**, ensuring a gradual increase in packing fraction and minimizing sudden disruptions in the system.

Pressure Measurement:

The compute stress/atom command was used to calculate the per-atom stress tensor, from which the overall pressure on the system was derived by just dividing by stress tensor tracer values by 2 (for 2D system).

Packing Fraction Calculation:

The change in vertical (y) distance between the moving walls was monitored to calculate the packing fraction. This was defined as the ratio of the total area occupied by particles to the area of the simulation box which is changing as the walls are moving.

3. Simulation Process:

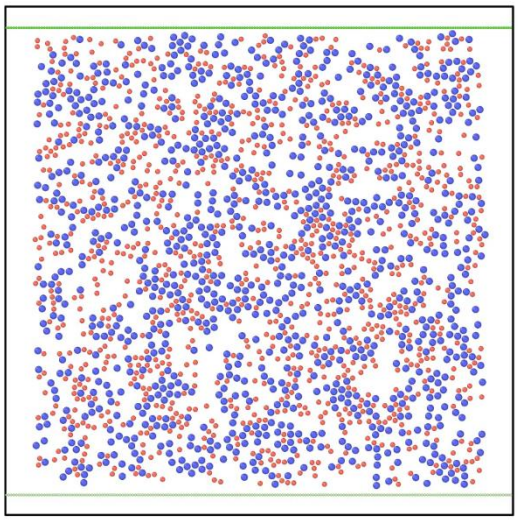
Compression Cycle:

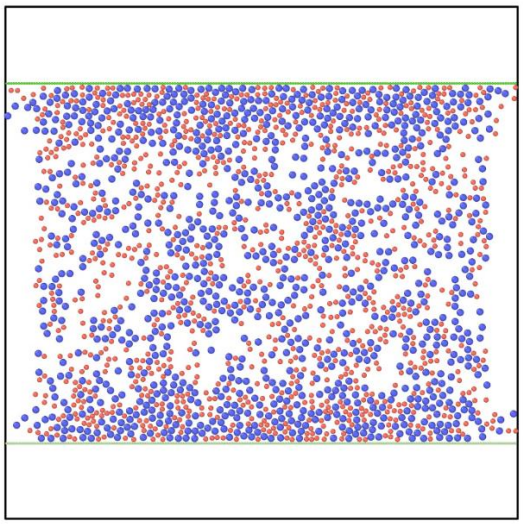
The fix move command was applied to gradually move the walls inward at a speed of 0.005, compressing the system and increasing the packing fraction up to approximately 0.83. During this phase, pressure data were collected using the compute stress/atom command.

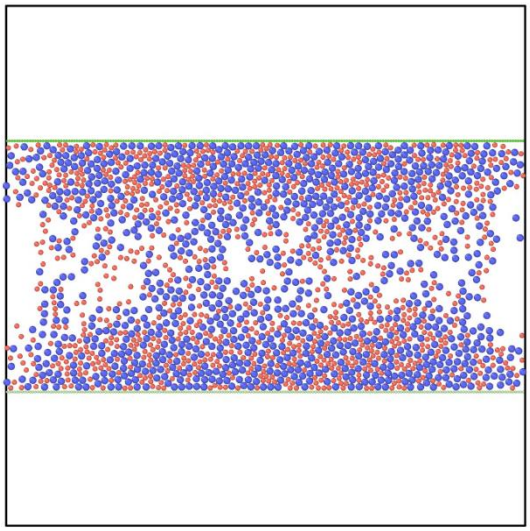
Decompression Cycle:

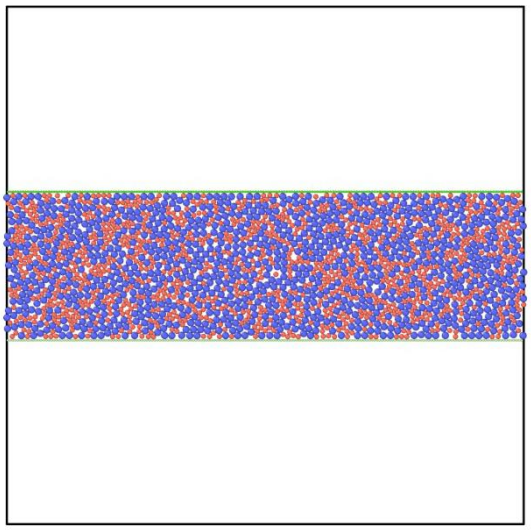
After reaching the target maximum packing fraction, the walls were moved outward, decompressing the system to lower the packing fraction. Pressure and wall position data continued to be recorded throughout this cycle.

4. Simulation Pictures:





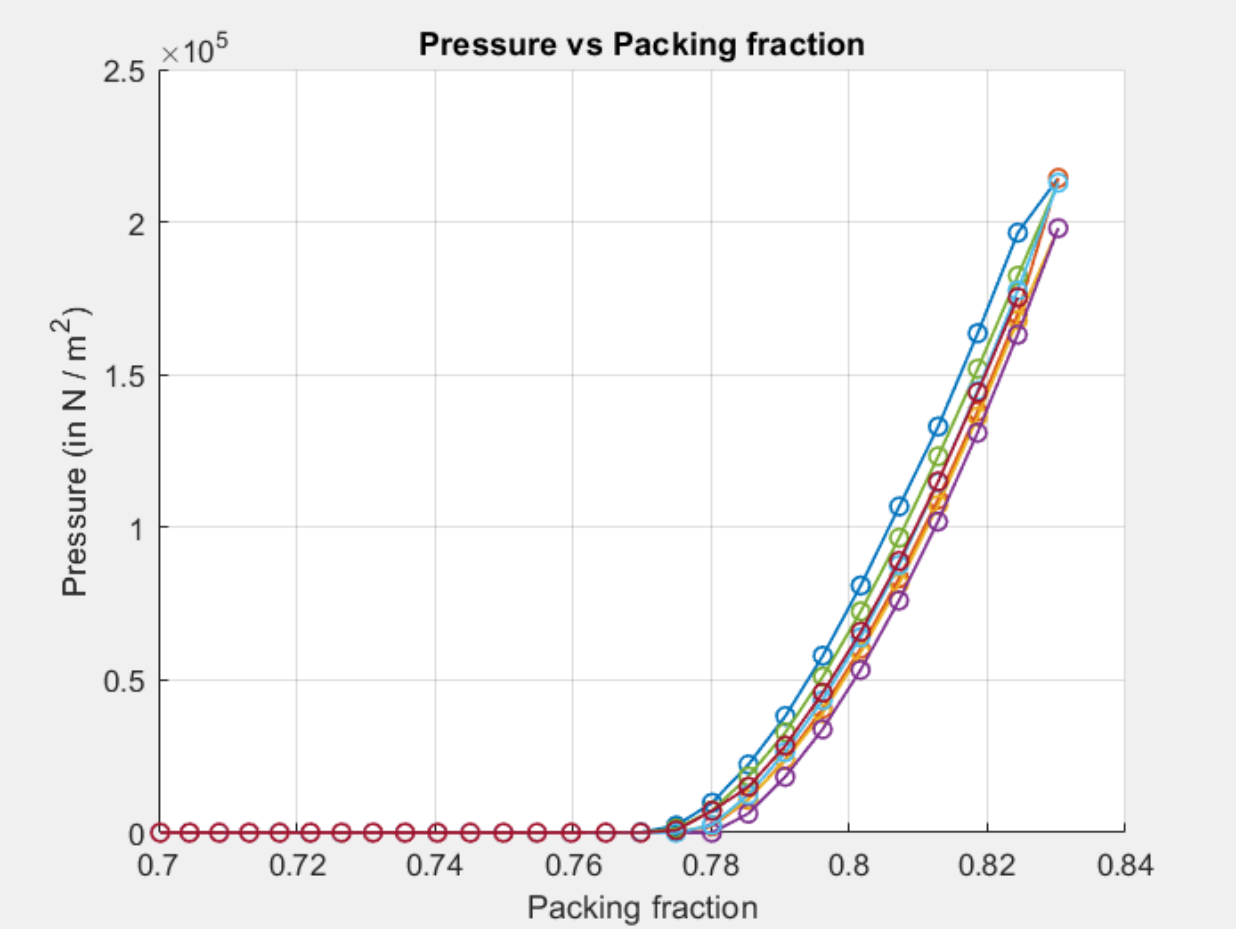




Data Analysis and Graph generation:

After all the data of pressure and packing fraction is generated for all the compression and decompression in LAMMPS, that data is processed using external script like MATLAB.

Whole data is converted in one csv file and having all the values of pressure corresponding to packing fraction, that csv file is used to plot the curve of Pressure v/s Packing fraction.



Result and Conclusion:

The simulation showed that pressure remained close to zero until the packing fraction reached approximately 0.77, after which it rapidly increased, reaching magnitudes on the order of 10^5 at a packing fraction of 0.83. This indicated that at lower densities, particle interactions were minimal, but beyond 0.77, the system became significantly more constrained, leading to a sharp pressure rise.

During the successive compressions and each decompression, the pressure did not return to its initial value, showing a slight decrease with each cycle and suggesting hysteresis in the system. The observed hysteresis, where the pressure after decompression did not match the initial compression values, points to energy dissipation and irreversible structural changes within the granular system. This behaviour could be explained by internal friction, particle rearrangements, and potential microstructural shifts during compression and decompression cycles and it implies that to reach the same peak pressure after decompression, further compression beyond 0.83 is needed, highlighting the irreversible nature of granular packing under repeated loading.

Difficulties Faced:

Major challenges during the simulation and data processing phases:

Simulation Time: The use of the fix viscous command, which is intended to relax the system at each step for more accurate pressure calculations, resulted in extremely long simulation times. Each compression cycle took more than 10 hours to simulate, which significantly slowed down the process and made it impractical to complete multiple iterations. That is why I was unable to use that. This made it difficult to explore different system configurations or conduct more extensive analysis within a reasonable time frame.

Data Handling and Exporting: The simulation generated a large volume of data, but due to the sheer size of the output, Excel was unable to export the entire dataset into a single CSV file. This limitation resulted in only a small subset of the data being used for graph generation. Although the simulation produced a lot of valuable data, the inability to process and visualize the full dataset limited the depth of analysis that could be presented.

References:

LAMMPS documentation

Training, memory and universal scaling in amorphous frictional granular matter - IOPscience