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Identifying Particle Interaction Features that Drive Clustering in Dense Suspensions

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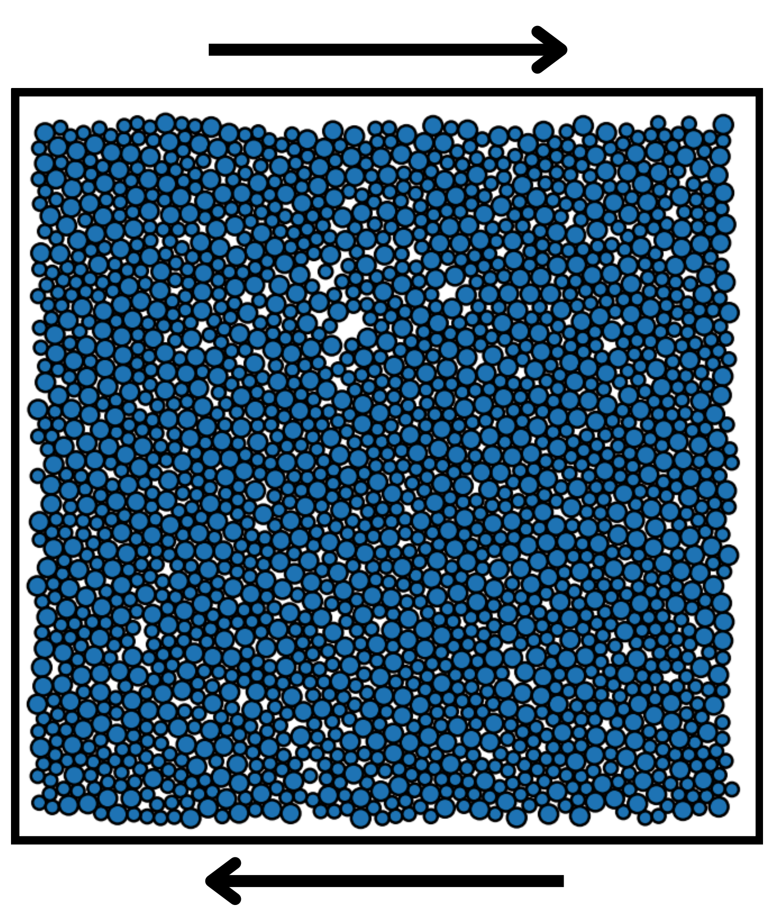
Introduction

Dense suspensions are mixtures of solid particles that are packed closely together in a fluid, and arise in many familiar materials like cement, mud, and cornstarch in water. In this work, we observe a 2-D dense suspension composed of rigid non-Brownian particles. As the shear stress increases, particle contact can transition from lubricated to frictional, temporarily forming **clusters** in which the particle arrangement cannot be changed without breaking contacts. This project analyzes dense suspension simulation data to identify particle specific or structural features that differentiate clustered and non-clustered particles.

Methodology

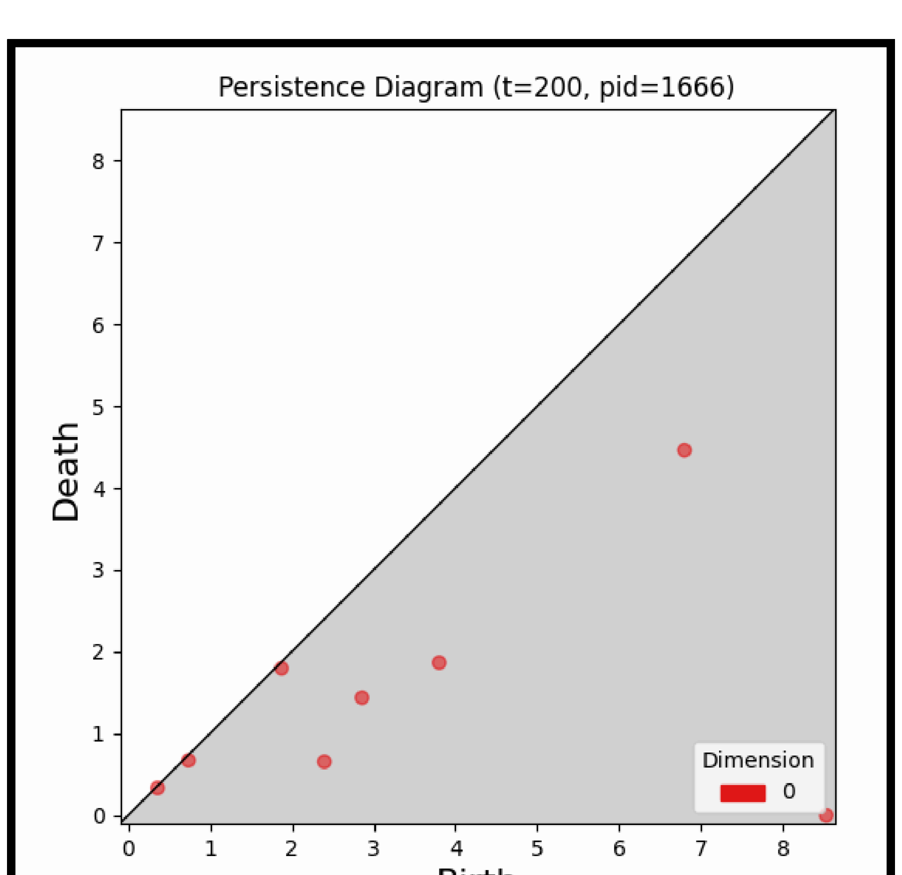
The simulation data was generated using the computational framework LF-DEM [2], which mimics dense suspension systems under hydrodynamic and frictional forces. In the simulations, 2000 particles of size 'a' and '1.4a' in equal proportion [1] are placed in a virtual shear cell (as seen below), where the top and bottom boundaries move in opposition to apply a shear stress. This system has a packing fraction of 0.76 (particles occupy 76% of the area). As the particles move and interact, the simulation calculates information such as their positions, velocities, angular velocities, and the forces between them. This forms a detailed record of the evolution of particle interaction within the contact network containing 2000 particles for each of the 1201 timesteps in a simulation for a single shear stress value (4 values in total are used, normalized by the lowest). After generating datasets using LF-DEM, the pebble game [3] was used to differentiate rigidly connected, clustered (structurally immovable) particles and non-clustered particles.



Swatch - Cloth Method

Particle contact in dense suspensions can be seen as a time-evolving network where each timestep forms a graph with particles as nodes and edges that represent (non - sliding and sliding) frictional contacts weighted by the normal forces between them. Such networks can be analyzed using topology, with one such approach is the swatch - cloth method [4]. A **swatch** is a small sub-network centered around a **particle** (node), extending out to four layers of contacts for neighboring particles.

Persistence diagrams allow for network topology to be measured using a weighting or threshold. These diagrams stem from persistent homology, a study that tracks the birth and death of topological features such as clusters, loops, and voids [1]. Persistence diagrams were generated for each of the swatches, using the **normal force** between the two particles as weighting.

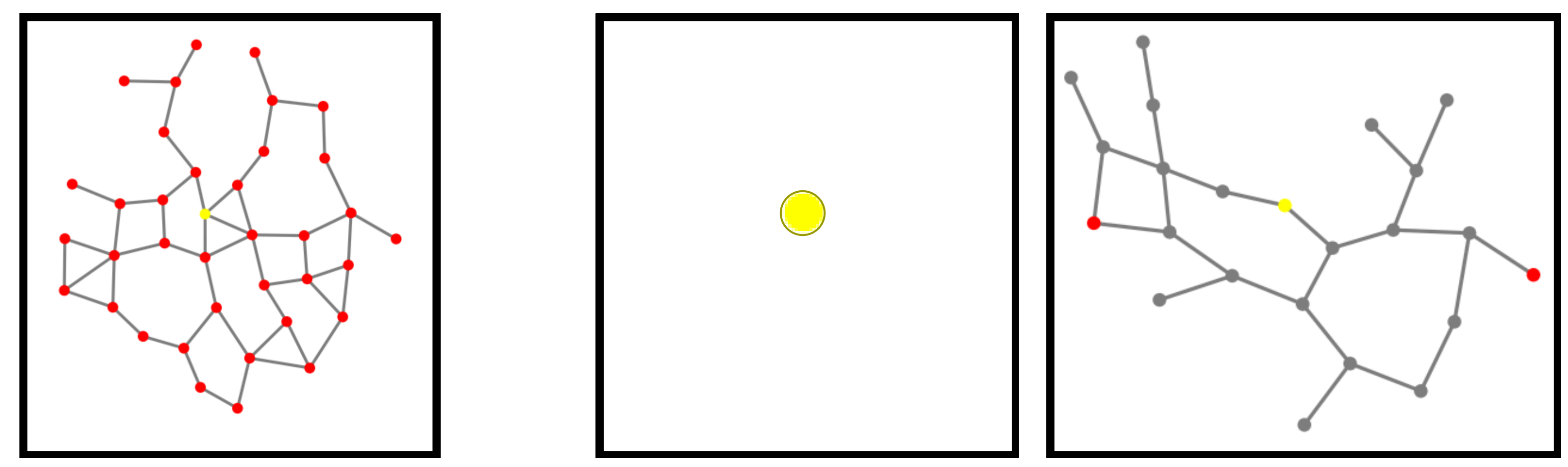


Persistence diagram of particle of index 1666 from timestep 166 under shear stress 5.

Results

Shown below are examples of swatches where the center particle (seen in yellow) is clustered or non-clustered. In the neighboring particles, the red particles are clustered while the grey particles are non-clustered.

Clustered Center | **Not Clustered Center**



The nodes in the graph depict particle placement, and the edge length is the distance from the center of one node to the center of the node it is in frictional contact with.

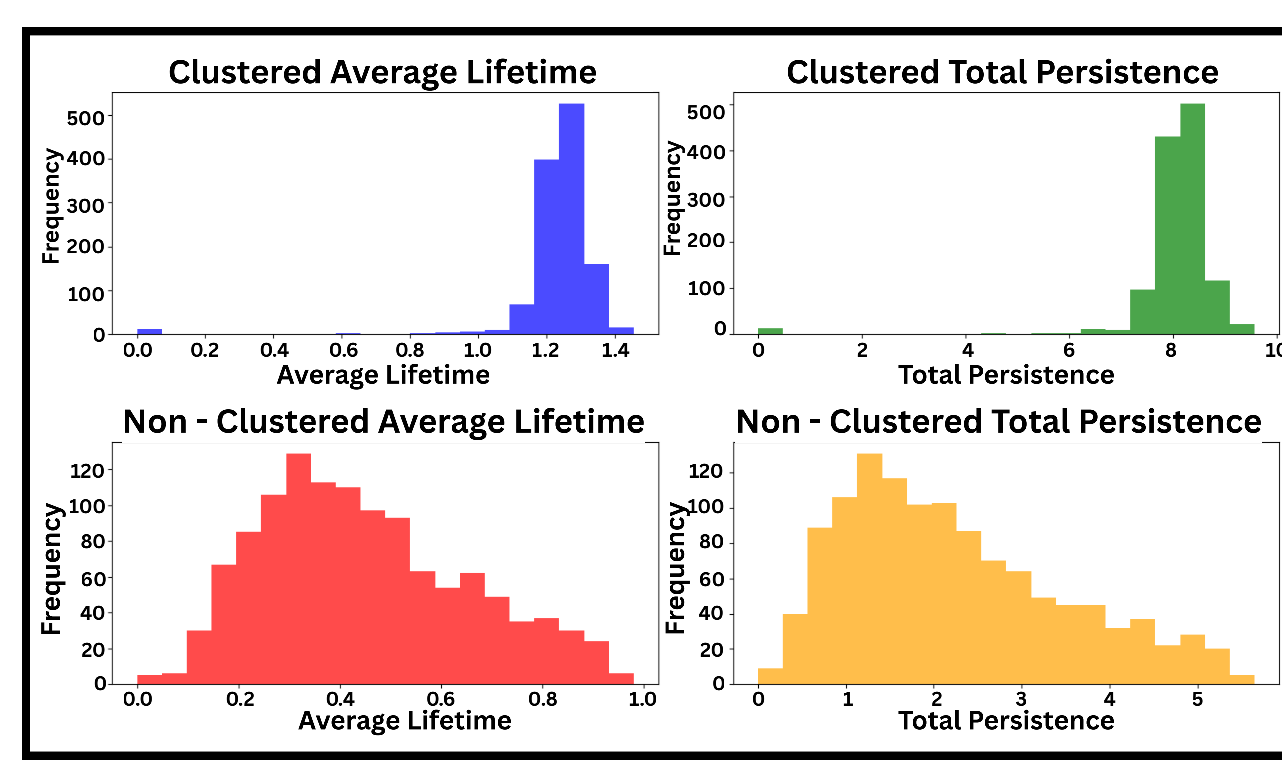
Particles with large, highly connected local networks tended to be part of clusters, while non-clustered particles either had smaller to medium sized networks or, in many cases, were isolated with no frictional contacts at all.

To see if the structural properties of a swatch could help classify particles as clustered vs. non-clustered, for each timestep, a Random Forest Classification model was trained using the number of particles per layer, particles per layer, the average degree per layer, and the standard deviation of the degrees per layer in each swatch, where each layer is composed of particles that are a certain number of hops away from the root particle.

Normalized Shear Stress	1	2	5	10
Average Accuracy over Timesteps	0.9998	0.9712	0.9224	0.9909

Average classification accuracy of differentiating clustered and non-clustered particles across all timesteps in a simulation for the shear stresses shown.

From each persistence diagram, two quantities were calculated to summarize the network's topological behavior. The **lifetime** of a feature was the difference between its birth and death values, and the **total persistence** of a diagram was obtained by summing the lifetimes of all its features. For each swatch in each timestep the average lifetime as well as the total persistence were calculated. The swatches were separated into clustered and non - clustered particles, and the average persistence statistics for both categories were found. These values were then calculated over each timestep and were used to create histograms exploring the frequency of both the mean (in a timestep) of the average lifetime (in a swatch) as well as the mean (in a timestep) of the total persistence.



Clustered particles (top row) display narrow, higher -valued distributions, as compared to non-clustered particles (bottom row) which show broader distributions shifted toward lower values.

Future Work

In the future, we plan to continue exploring the frictional contact networks using the swatch–cloth framework, which has proven effective for capturing local structural organization in dense suspensions. We plan to extend this analysis from two-dimensional simulations to fully three-dimensional systems in order to examine whether the same network features distinguish clustered from non-clustered particles.

References

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