Research and Creative Experience for Undergraduates Program (RCEU) Summer 2021

The Effect of Surface Topography on the Deposition of Colloids

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Introduction

The roughness of a surface is significant in many facets such as "Paints, water-proof clothing, non-stick cookware, adhesives, and anti-glare lenses" [1]. The roughness is determined by a surface's topography. Understanding and control of certain properties of adhesion from these surfaces can influence the usages of these surfaces.

Methodology

We run Monte Carlo Simulations for 600,000 steps to equilibrate the system. The initial configuration is shown in Figure 1, with a fix number of particles set to 1000. We consider periodic boundary conditions along the horizontal axis, and a reflective boundary top. Furthermore, the ellipsoids were aligned on the bottom surface to simulate a surface roughness. The roughness is varied based on the dimensionless separation distance between ellipsoids, using the particle radius $r_x = r_m$ as a reference, as shown in Figure 2. The dimensionless distances between ellipsoids were set to $\delta_s = 0.3$, 1, and 1.6.

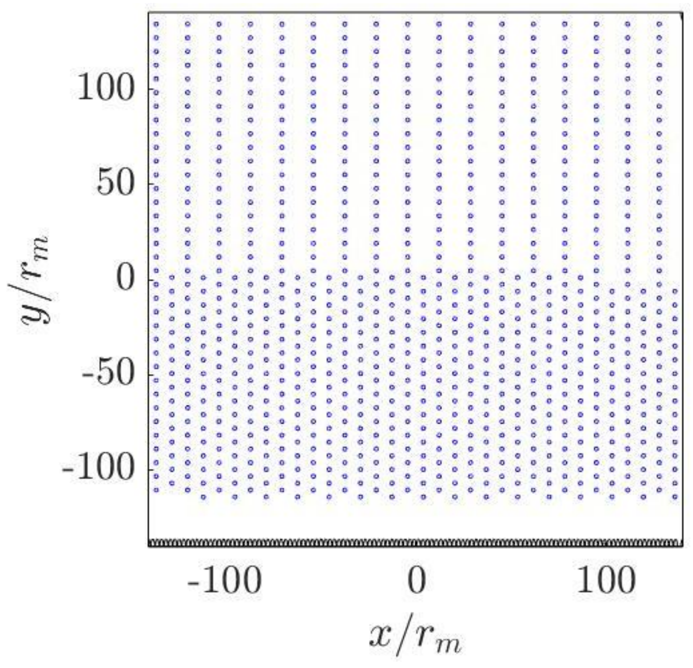

Figure 1. Initial configuration of the spherical particles over the rough surface. 1000 particles are present. The ellipsoids have an aspect ratio $r_y/r_x = 4$

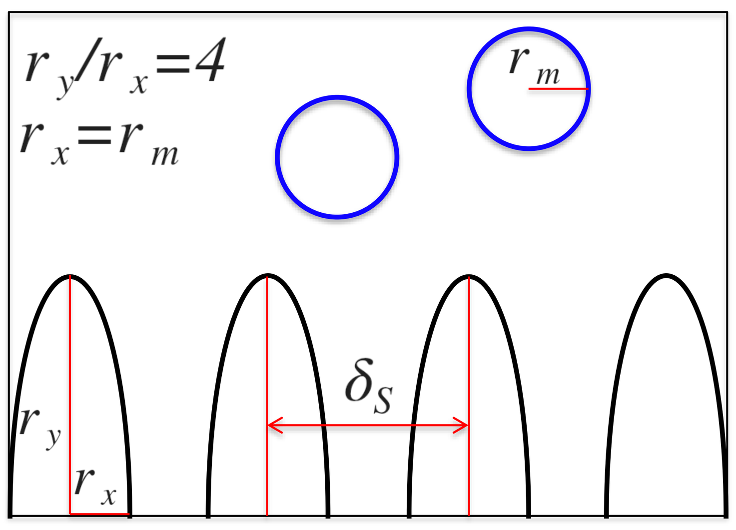

Figure 2. A schematic representation of the rough surface used for simulations.

We use a Derjaguin approximation to model the repulsive interaction between spheres in suspension and between spheres and ellipsoids. We model the ellipsoid with the equivalent sphere at the end of the ellipsoid, as shown in Figure 3.

$$U_e = \left(\frac{R_1 R_2}{R_1 + R_2} \right) Z e^{-\kappa D}$$

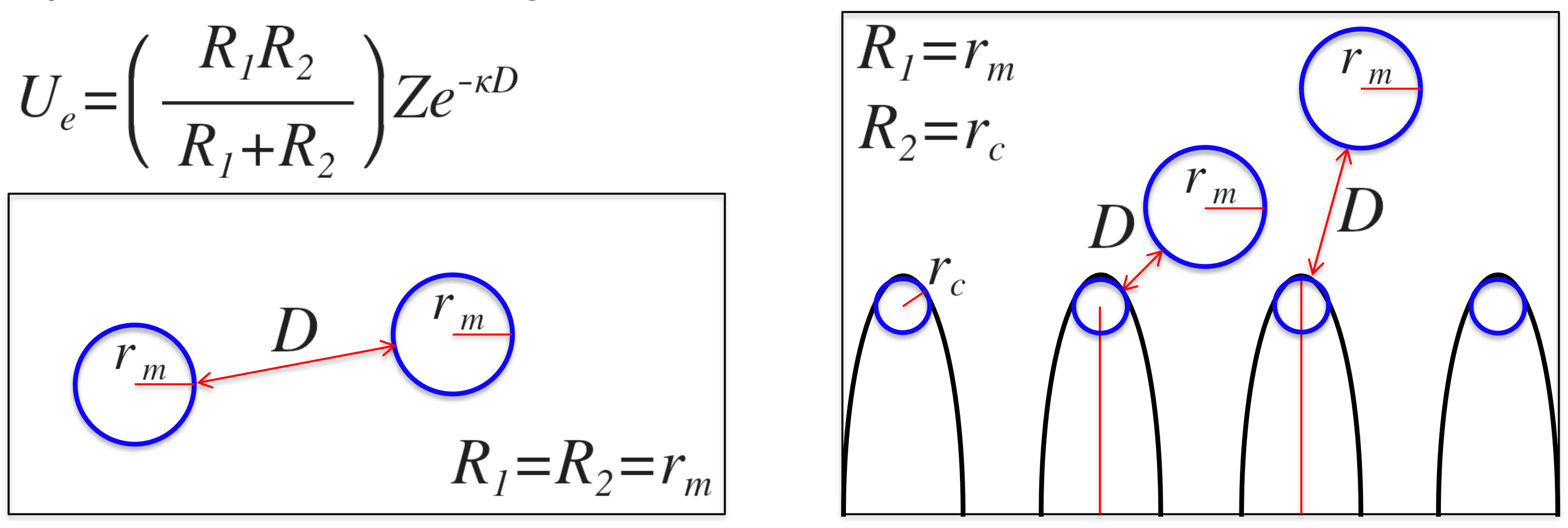

Figure 3. Schematic shows the distance at which the repulsive interaction was calculated over and the radii used for this. The equation is applied to both circles and ellipses in the simulation [2].

Results

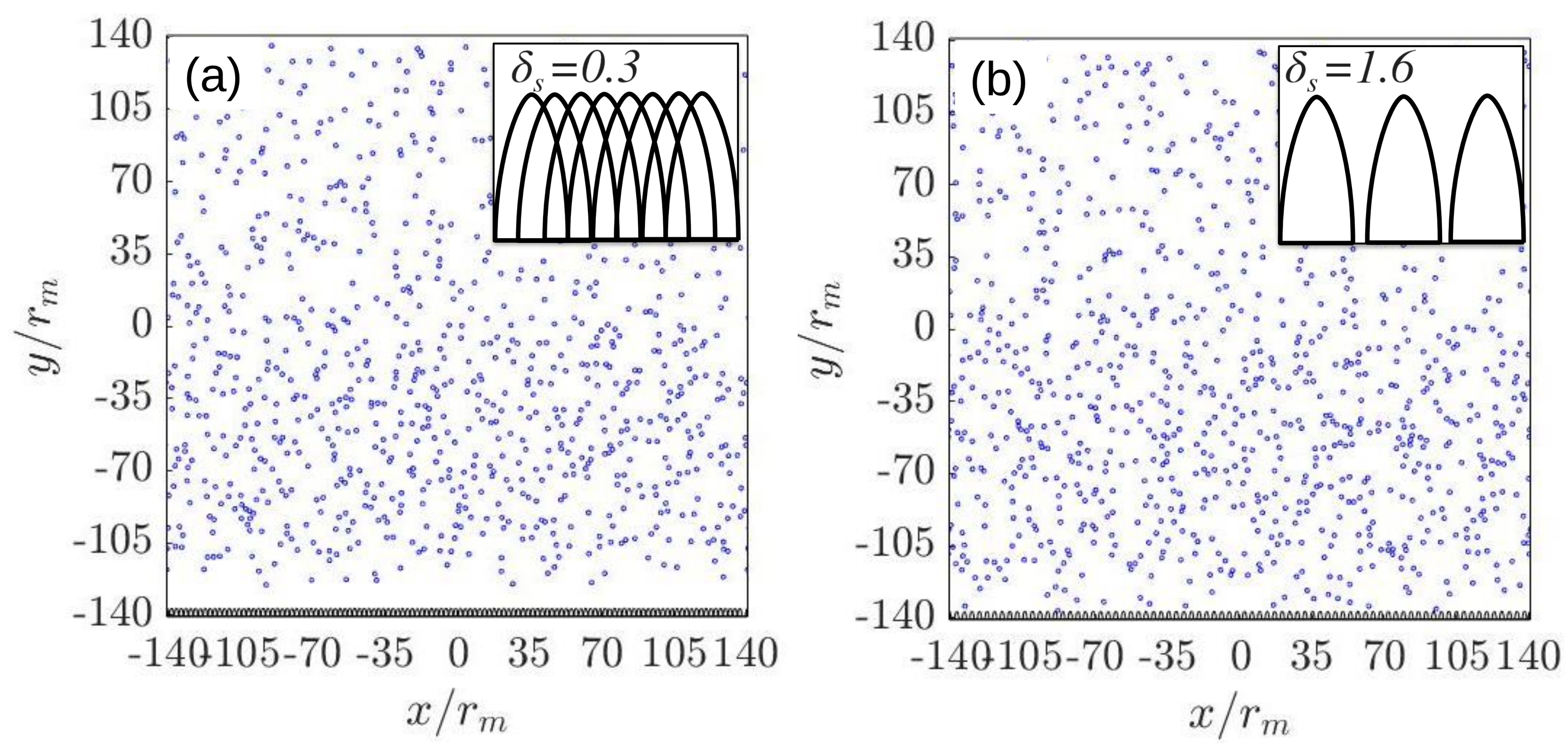

Figure 4. Snapshots of the simulation of spheres without gravitational potential. (a) Shows a separation distance of $\delta_s = 0.3$ and (b) shows $\delta_s = 1.6$.

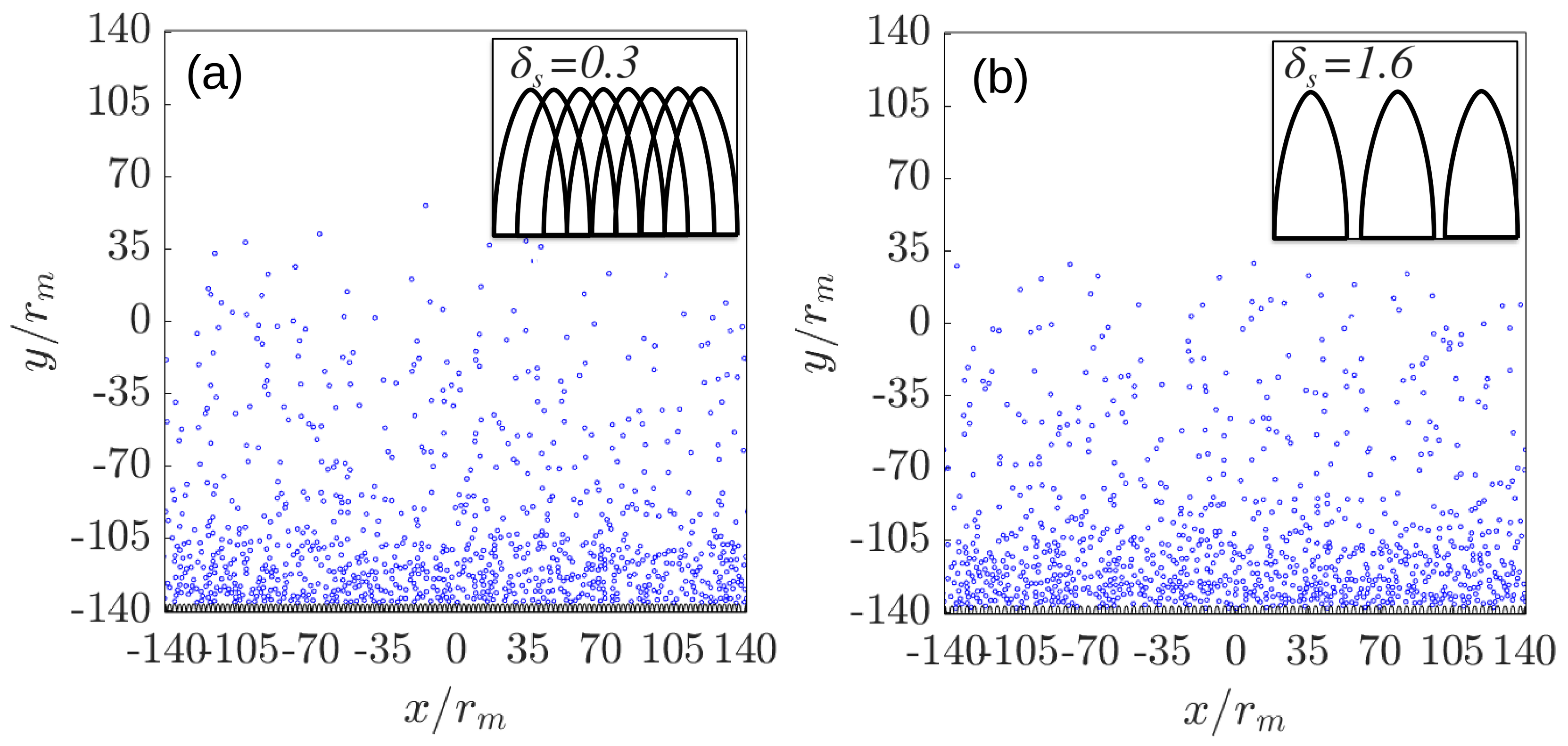

Figure 5. Snapshots of the simulation of spheres with gravitational potential interacting with the rough surface. (a) Shows a separation distance of $\delta_s = 0.3$ and (b) shows $\delta_s = 1.6$.

Conclusions and Future Work

We develop a model to study the particle interaction between spheres and a ellipsoid surface. The model includes repulsive interaction of the ellipsoids and spheres, gravity, and Monte Carlo equilibration. The preliminary results show that the particle deposition decreases as the roughness separation increases.

Future steps include developing a 3-dimensional analysis of the particle deposition on rough surfaces. Additionally, it will include the interaction energy as a function of position and orientation superellipsoidal particles.

References

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2. Israelachvili, J. N. (2012). Electrostatic Forces between Surfaces in Liquids. In *Intermolecular and surface forces*. essay, Academic Press is an imprint of Elsevier.

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