Simulation and Modeling
Project I: Molecular Friction

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1 Introduction

As suggested in Gould's book (pp. 279-280), I adapted Ringlein & Robbins' simulation of a microscopic model of friction for python and performed similar analysis to reach an independent reproduction of those results; namely, that the coefficient of friction increases linearly with effective area A_{eff}, where A_{eff} is a measure of the molecular contact region. In these simulations, A_{eff} is modified in by modifying the normal force acting upon each particle in the sled. The results show that the force it takes to pull the sled over the initial trough increases as a linear function of A_{eff}, matching Ringlein & Robbins' results.

2 Method

I implemented a simulation in python which used the Verlet integration method and a collection of forces (Lennard-Jones, normal, spring, pulling, damping) to advance a container of particles through time. The particles were segregated into floor particles (which received no resultant acceleration) and sled particles (which were connected by springs in a triangular truss, wide side down). In each time step, particles in the sled experienced an all-pairs Lennard-Jones interaction, a normal force (positive or negative), and spring interactions with connected particles. Additionally, the puller (farthest right sled particle) was forced right at a constant rate by a separate spring interaction, while the damper (farthest left sled particle) experienced a force proportionally opposed to its velocity. The state data (positions, velocities, and accelerations) for each particle were stored, along with metadata describing the varying force coefficients, in a time-stamped container and aggregated to create animations of the particles' positions over time as well as plots of forces.

To validate Ringlein & Robbins' conclusions, it was necessary to track the pulling force, F_p, as it changed over time. Then the friction force was interpreted as the peak force experienced before the sled left its trough (i.e. moved by more than $a = \frac{1}{2}2^{\frac{1}{6}}$).

3 Verification of Program

Previous work showed, through conservation of energy and visual inspection, that the Lennard-Jones force between particles was correctly implemented (importantly, an integration dt of 0.01 was found to be adequate). Further, visual inspection and live-updating of values in animations were used to verify that the damping and pulling forces were (at least qualitatively) correct. Finally, results closely matching Ringlein & Robbins' imply conformance.

4 Data

I determined the frictional force for each system described in the following table.

N	μ_s	c
1	0.417	2.726
9	0.397	2.234
13	0.383	2.193
17	0.366	2.146

N is the number of particles in the sled. W varied from -20 to 40 by increments of five (except for N=1, which started at W=0). Pulling rate (F_{pv}) was 0.1. Coefficients are a least-squares fit to the equation $f_s = \mu_s W + cA_{eff}$ where A_{eff} is the number of sled particles in contact with the floor.

The pulling force of a particle was plotted vs time to show the pattern of peaking indicative of static friction (Figure 1).

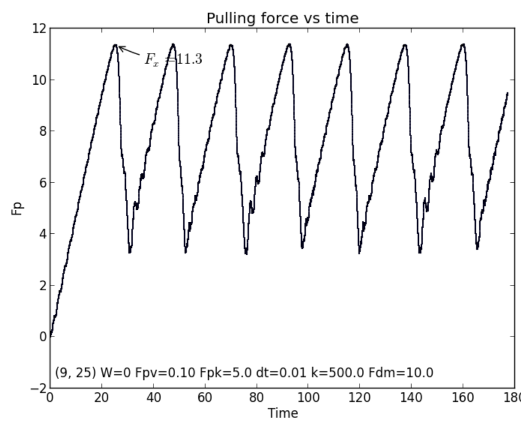

Figure 1: A lengthy run of the simulation shows that the pattern of increasing the pulling force until a breaking point is reached is periodic.

Figure 2 replicates Ringlein & Robbins' (p. 886) plot of friction force vs normal force for a variety of sled sizes.

A comprehensive view of friction force vs time for varying normal forces and sled sizes is shown in Figure 3.

5 Analysis

It is clear from Figure 2 that the friction force changes linearly with respect to normal force, regardless of the sled size. Since the normal force is increasing the proximity of contact between the sled and the floor, it can be thought of as an increase in A_{eff}.

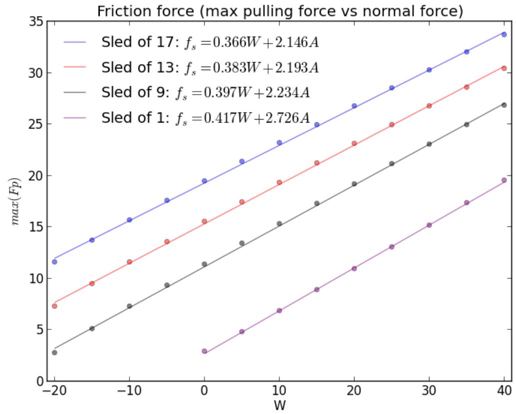

Figure 2: A plot of $max(Fp)$ vs normal force for several sled sizes, as well as linear least-squares fits, show that the coefficient of friction and area multiplier vary a bit.

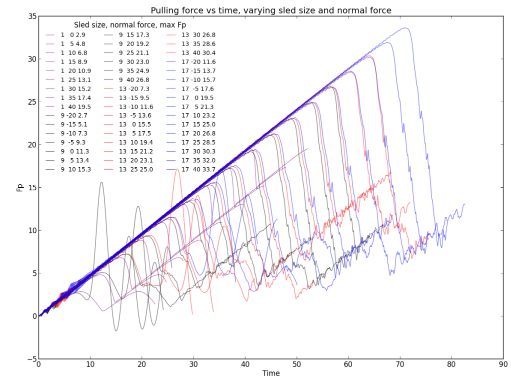

Figure 3: Comparing Fp vs time for all sled sizes and normal forces shows how similar each simulation run is. Note the erratic oscillations in the early times - these were due to negative normal forces causing the sled to fly away after exceeding f_s.

6 Interpretation

I do not know why the values of μ_s and c vary with sled size (as opposed to Ringlein & Robbins' constant values of $\mu_s = 0.308$ and $c = 1.96$ (p. 886). Ringlein & Robbins do not detail how the normal force in their simulation is applied, and I took Gould's suggestion of assigning the value W/N to each sled particle (N being the number of sled particles). However, this results in different normal forces per particle for the same value of W but varying sled sizes. Nonetheless, the values obtained for μ_s do not differ significantly from Ringlein & Robbins'.

7 Critique

The Interactive Physics software used by Ringlein & Robbins is not familiar to me, so I do not know whether or not my simulation provided more accurate or less accurate data. Ringlein & Robbins do not discuss the time step used by their software, and I settled on a value found to be sufficient for previous work that may not have been precise enough for this simulation.

Additionally, some of the system parameters described by Gould (pulling rate, spring constants, etc) were not the same as those used by Ringlein & Robbins, and in some cases I chose to use entirely different values. These discrepancies certainly contributed to the differing results.

References

[1] Gould, H., Tobochnik, J., & Christian, W. (2007). *An Introduction to Computer Simulation Methods: Applications to Physical Systems*. San Francisco, CA: Pearson Education, Inc.

[2] Ringlein, J. & Robbins, M. *Understanding and illustrating the atomic origins of friction*. Am. J. Phys. 72, 884 (2004); doi: 10.1119/1.1715107