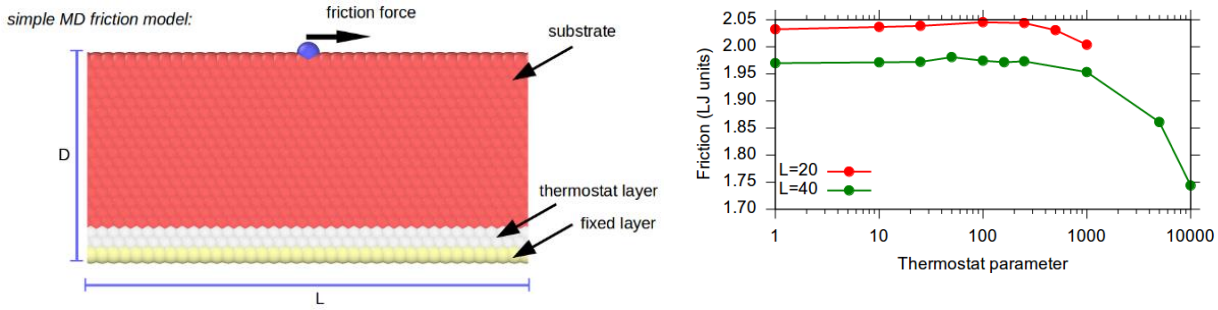
High resolution molecular dynamics simulations of friction

Friction is one of the major causes of energy loss in the industrialized world. It is therefore remarkable that many frictional phenomena still remain poorly understood. Even for a very simple theoretical friction model (left figure), consisting of a single particle being dragged over a substrate in a molecular dynamics (MD) simulation, the friction force cannot be unambiguously determined.



There are several reasons for this:

(1) The friction that you measure depends on the sizes (L and D) of the model. The effect is visible as the difference between the red and green curves in the right graph (which were both obtained for the same value of D). Comparing to experiments, where L and D are typically much larger than what can be reached in simulations, is therefore difficult.

(2) More seriously, the friction force depends on how you control the temperature in the simulation. Temperature is typically controlled in these simulations using a thermostat attached to the bottom of the system. As the green curve shows, by varying the thermostat parameter, one can basically get the friction to become arbitrarily small, even though the temperature of the heat bath is the same for all points on the curve!

The aims of this Master project are 2-fold:

First, by performing simulations for various system sizes L and D, we want to derive scaling laws that would enable us to estimate friction in a large system based on simulation data obtained in smaller systems.

Second, the influence of the thermostat needs to be carefully elucidated. The working hypothesis here is that thermostats “filter out” lattice vibrations from the substrate only of certain wavelengths and frequencies. Hence, each thermostat removes the energy from the system in its own way, which is why the friction that you measure depends on the thermostat that you use.

In this Master project, besides studying friction, you will also learn about using high-performance computing hardware. If you enjoy computers and programming then that would be an added bonus! In addition, exciting friction AFM experiments are performed in our institute. The results obtained in this project serve as a prerequisite toward modeling these experiments.

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