

Title

Subtitle

by

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for the degree of

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Faculty of Mathematics and Natural Sciences  
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Title

Subtitle

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# Abstract

Abstract.





# Acknowledgments

Acknowledgments.



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# List of symbols?

Maybe add list of symbols and where they are used like Trømborg.



# Introduction

## 0.1 Motivation

### 0.1.1 Friction

Friction is a fundamental force that takes part in almost all interactions with physical matter. Even though the everyday person might not be familiar with the term “friction” we would undoubtedly notice its disappearing. Without friction, it would not be possible to walk across a flat surface, lean against the wall or secure an object by the use of nails or screws (Static friction allows us to join objects together using screws [1][p. 5]). Similarly, we expect a moving object to eventually come to a stop if not supplied with new energy, and we know intuitively that sliding down a snow covered hill is much more exciting than its grassy counterpart. It is probably safe to say that the concept of friction is well integrated in our everyday life to such an extent that most people take it for granted. However, the efforts to control friction dates back to the early civilization (3500 B.C.) with the use of the wheel and lubricants to reduce friction in translational motion [2]. Friction is a part of the wider field tribology derived from the Greek word *Tribos* meaning rubbing and includes the science of friction, wear and lubrication [2].

The most important motivation to study tribology is ultimately to gain full control of frictional and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages regarding energy efficiency. It has been reported that that monetary value of tribological problems has significant potential for economic and environmental improvements [3]:

“On global scale, these savings would amount to 1.4% of the GDP annually and 8.7% of the total energy consumption in the long term.” [4].

The reduction of friction is not the only sensible application as a controlled increase in friction might be of interest in the development of grasping robots or perhaps braking system (get some sourced examples maybe...).

To the best of my knowledge kirigami has not yet been implemented to alter the friction properties in a similar manner as done in this thesis.

### 0.1.2 Thesis

In this thesis we investigate the possibility to control the frictional properties of a graphene sheet by applying strategically positioned cuts to the sheet inspired by kirigami. Kirigami is a variation of origami where the paper is cut additionally to being folded. Hanakata et al. [5] has shown that kirigami inspired cuts on a graphene sheet can be used to alter the yield strain and yield stress of the sheet. They observed that the stretching of the cut sheet induced a out-of-plane buckling which serves as a key observation for the motivation of this thesis. It is currently well established/believed that the friction between two surfaces is proportional to the real microscopic contact area (source here?). Hence, one can hypothesize that the buckling of the sheet will affect the contact area and consequently the frictional properties.

## 0.2 Approach

In the study by Hanakata et al. [5] they used a machine learning (ML) approach to overcome the complexity of the nonlinear effects arising from the out-of-plane buckling which made them successfully map the cutting patterns to the mechanical properties of yield and stress. The dataset used for the ML training was generated by molecular dynamics (MD) simulations for a limited set of cut configuration. By training the network the

MD simulations could effectively be skipped all together making for an accelerated search through new cut configurations for certain mechanical properties. By setting up a MD simulation that quantifies the frictional properties of the graphene sheet we aim to make an analog study regarding the search for certain frictional properties.

We will take this one step further by creating a GAN network that utilises the latter network for creating an inverse design framework. That is, a network that takes frictional properties as input and return the corresponding cut configuration. By having such a tool we can execute a targeted search for exotic frictional properties. Particularly, we are interested in nonlinear and possibly even negative friction coefficients. Friction is essentially observed to increase with increasing load on the frictional surface, and we often describe this as having a positive friction coefficient. However, if we are able to couple the stretching of the sheet with friction we might be able to break this barrier for the coefficient. By imagining some nanomachine which translates downward pressure into either compression or expansion of the altered graphene, we could have a coupling between downward pressure and stretch of the sheet. In that case, a friction force depending on stretch could effectively be made to decrease with increasing load which would correspond to a negative friction coefficient following this definition (formulate such that we do not imply free acceleration from nothing).

One of the features from inverse design, separating it from the general class of ML approaches, is that we do not depend on trusting the ML predictions. While a standard neural network might be extremely efficient on a certain prediction task we have usually no information on how these predictions are based. We say that the internal workings of the network is a black box beyond our capacity of interpretation. However, for the inverse design problem we are prompted with a few promising design proposals which can immediately be tested in the MD simulations which we will regard as the most reliable predictor in this setting. Hence, if arriving at a successful design in alignment our search prompt, we can disregard any uncertainty in the network. In that case the remaining gap to bridge is that of the MD simulation and real life implementations.

### 0.3 Objective of the study

1. Design a MD simulation to evaluate the frictional properties of the graphene sheet under different variations of cut patterns, stretching and loading, among other physical variables.
2. Train a network to replace the MD simulation completely.
3. (Variation 1) Do an accelerated search using the ML network for exotic frictional properties such as low and friction coefficients and a strong coupling between stretch and friction.
4. (Variation 2) Make a GAN network using the first network and predict cut configurations for some of the above mentioned frictional properties.
5. (If I have time) Make a nanomachine that couples load and stretch (perhaps just artificially without any molecular mechanism) to test the hypothesis of a negative friction coefficient.

### 0.4 Contributions

What did I actually achieve

### 0.5 Thesis structure

How is the thesis structured.



# Simulations

## 0.6 Baseline study (find better name)

Consider relabeling drag length to sliding distance instead.

### 0.6.1 Friction simulation parameters

The friction simulation is governed by a set of parameters where some is kept constant while other is varied to gain insight in the frictional properties. These parameters can be categorised into three main categories of different purpose as described in table [1](#).

**Table 1:** Parameters of the numerical procedure for measuring friction.

Category	Parameter name: description	Category purpose
Physical	<ul style="list-style-type: none"> <li>- <math>T</math>: Temperature for the Langevin thermostat.</li> <li>- <math>v_{\text{slide}}</math>: Sliding speed for the sheet translation.</li> <li>- <math>K</math>: Spring constant for the spring force between the virtual atom and the pull blocks responsible for translating the sheet along the substrate. An infinite spring constant is achieved by moving the pull blocks as a rigid body (Lammps: fix move).</li> <li>- Scan angle: The direction for which we translate the sheet.</li> </ul>	Parameters expected to have a physical effect on the friction properties, which is kept fixed and thus not included in the machine learning input set.
Measurement	<ul style="list-style-type: none"> <li>- <math>dt</math>: Integration timestep.</li> <li>- <math>t_R</math>: Relaxation time before stretching.</li> <li>- Pauses between stretch and adding normal force and between dragging the sheet.</li> <li>- Stretch Speed: How fast to stretch the sheet.</li> <li>- Slide distance: How far to translate the sheet.</li> <li>- Sheet size: Spatial size of the 2D sheet.</li> <li>- Pull block size: spatial size of the pull blocks.</li> </ul>	Parameters influencing the simulation dynamics and being representative of the experimental procedure that we are mimicking. These parameters are chosen with the aim of getting stable parameters under small perturbations of the given parameter.
ML input	<ul style="list-style-type: none"> <li>- Sheet configuration: A binary matrix containing information of which atoms are removed (0) and which are still present (1) in the graphene sheet.</li> <li>- Stretch amount: The relative sheet stretch in percentage.</li> <li>- <math>F_N</math>: Applied normal force to the pull blocks.</li> </ul>	The remaining parameters serve as input variables for the optimization process and are thus given as input variables for the machine learning (ML).

Due to the great number of parameters, and corresponding range of reasonable numerical values they can take, it is ... to parameter search including all of these. Thus, we will to a great extent rely on a reverse engineering in order to establish a set of parameters for the *physical* and *measurement* categories along with numerical ranges for the *ML input* category which gives stable and promising results. By doing so we effectively narrow down the parameter regime for which the investigated frictional properties belong. We aim to choose the parameters in order to accommodate a balance between generalizable and stable result which is simultaneously a suitable candidate as a proof of concept for the control of friction properties using kirigami inspired cuts.

In the following we present the results of the friction simulations in parallel to the procedure of investigating the choice of different parameters.

In the following subsections (X to Y) we are going to present the friction simulation results in parallel to the presentation of the reasoning behind the parameter choices. For this we will refer to the default parameter choice showcased in table 2 which is representative of the final parameter choices.

**Table 2:** Final parameters for the friction simulations **Probably not the neatest format for this...**

Physical	Measurements	ML input
$T = 300 \text{ K}$ $v_{\text{slide}} = 20 \text{ m/s}$ $K = \text{inf (LAMMPS: fix move)}$ Scan angle : $(x, y) = (0, 1)$	$dt = 1 \text{ fs}$ $t_R = 15 \text{ ps}$ Pauses = 5 ps Stretch speed = $0.01 \text{ ps}^{-1}$ Slide distance = $400 \text{ \AA}$ Sheet size = $130.029 \times 163.219 \text{ \AA}$ Pull block size = $2 \times 130.029 \times 15.183 \text{ \AA}$	Sheet configuration = Contiguous Stretch amount = Below rupture $F_N = [0.1, 10] \text{ nN}$

Say something about how these parameters is chosen. Reference to articles for which these was mirrored from.

#### 0.6.1.1 Pressure reference for normal load domain

Find place to put this.

In order to relate the magntidue of the normal force in our friciton measurement we will use the pressure as a reference. We will use the pressure underneath a stiletto shoe as a worst case for human pressure execution underneath the shoes. From (source 1) it is reported that the diameter of a stiletto heeled shoe can be less than 1 cm. Hence a 80 kg man<sup>1</sup> standing on one stiletto heel (with all the weight on the heel) will result in a pressure

$$P = \frac{F}{A} = \frac{mg}{r^2\pi} = \frac{80 \text{ kg} \cdot 9.8 \frac{\text{m}}{\text{s}^2}}{(\frac{1 \times 10^{-2} \text{ m}}{2})^2\pi} = 9.98 \text{ MPa}$$

While this is in itself a spectacular realization that is often used in introductory physics courses (source 2) to demonstrate the rather extreme pressure under a stiletto heel (greater than the foot of an elephant) (how many Atmos?) this serves as a reasonable upperbound for human executed pressure. With a full sheet area of  $\sim 21 \times 10^3 \text{ \AA}^2$  we can achieve a similar pressure of  $\sim 10 \text{ MPa}$  with a normal force of

$$F_N = 10 \text{ MPa} \cdot 21 \times 10^{-17} \text{ m}^2 = 2.10 \text{ nN}$$

Of course this pressure might be insufficient for various industrial purposes, but with no specific procedure in mind this serves as a decent reference point. Notice that if we consider a human foot with ares  $113 \text{ cm}^2$  the pressure drops to a mere  $70 \text{ kPa}$  corresponding to  $\sim 0.01 \text{ nN}$ .

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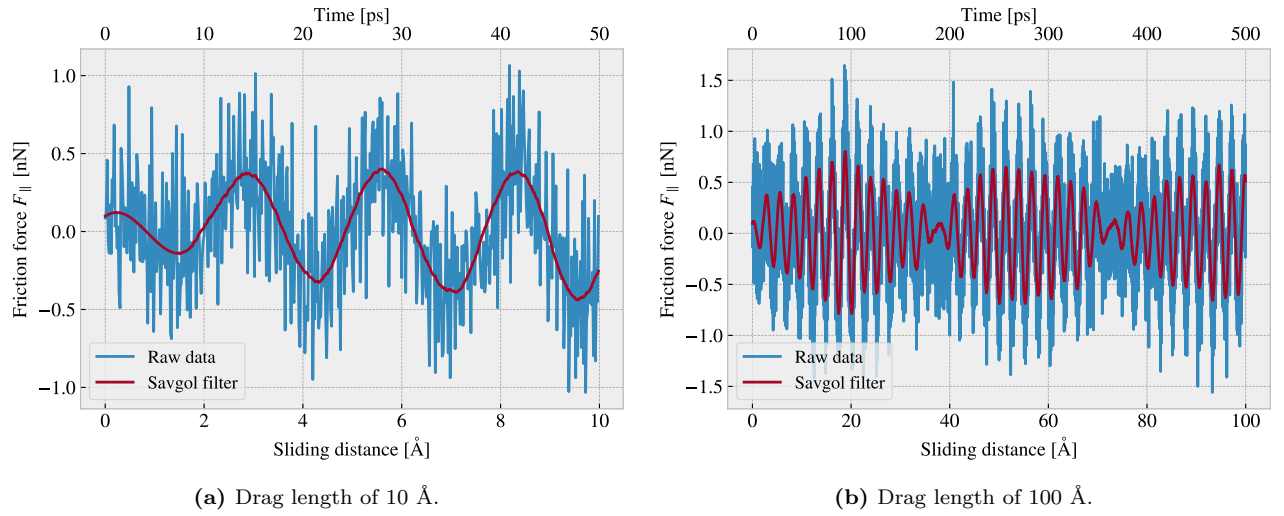
<sup>1</sup>Yes, a man can certainly wear stilleto heels.

## 0.6.2 Single friction simulation analysis

We begin by assessing the raw data for a single friction simulation run with the default parameters shown in table 2 for a non-cut sheet, no stretch and an applied normal force of 1 nN.

### 0.6.2.1 Force oscillations

We first assess the raw data for the friction force  $F_{\parallel}$  parallel to the drag direction as seen in figure 1. The sample rate is  $10 \text{ ps}^{-1} = 100 \text{ timesteps}^{-1}$  for which each sample is the mean value of the 100 timesteps preceding the given sample interval. We observe immediately that the data carries oscillations on different time scales. By applying a savgol filter to the data with a polyorder of 5 and window length of 150 timesteps, corresponding to a sliding distance of  $3 \text{ \AA}$  or a time window of 15 ps, we can qualitatively point out at least two different frequencies of oscillation. On figure 1a we see roughly three waves on the savgol filter corresponding to a relative high frequency, while on 1b the same savgol filter reveals a lower frequency on top of the first, creating the visual pattern of a wavepacket.



**Figure 1:** Friction force  $F_{\parallel}$  with respect to the drag direction between (full) sheet and substrate versus sliding distance. The sliding distance is measured by the constant movement of the virtual atom and not the COM of the sheet. However, we expect these measures to be fairly identical due the fact that the pull blocks is rigidly coupled to the virtual atom. The red line represents a savgol filter with window polyorder 5 and window length of 150 timesteps (corresponding to a sliding distance of  $3 \text{ \AA}$  or a time window of 15 ps).

By performing a Fourier Transform (FT) on the data we can quantify the leading frequencies as seen in figure 2a. By plotting the two most dominant frequencies  $f_1 = 0.0074 \text{ ps}^{-1}$  and  $f_2 = 0.0079 \text{ ps}^{-1}$  as  $\sin(2\pi f_1) + \sin(2\pi f_2)$  we find a qualitatively convincing fit to the observed wavepacket shape as seen in figure 2b. By using the trigonometric identity

$$\begin{aligned}\sin(\alpha + \beta) &= \sin(\alpha) \cos(\beta) + \cos(\alpha) \sin(\beta), \\ \sin(\alpha - \beta) &= \sin(\alpha) \cos(\beta) - \cos(\alpha) \sin(\beta),\end{aligned}$$

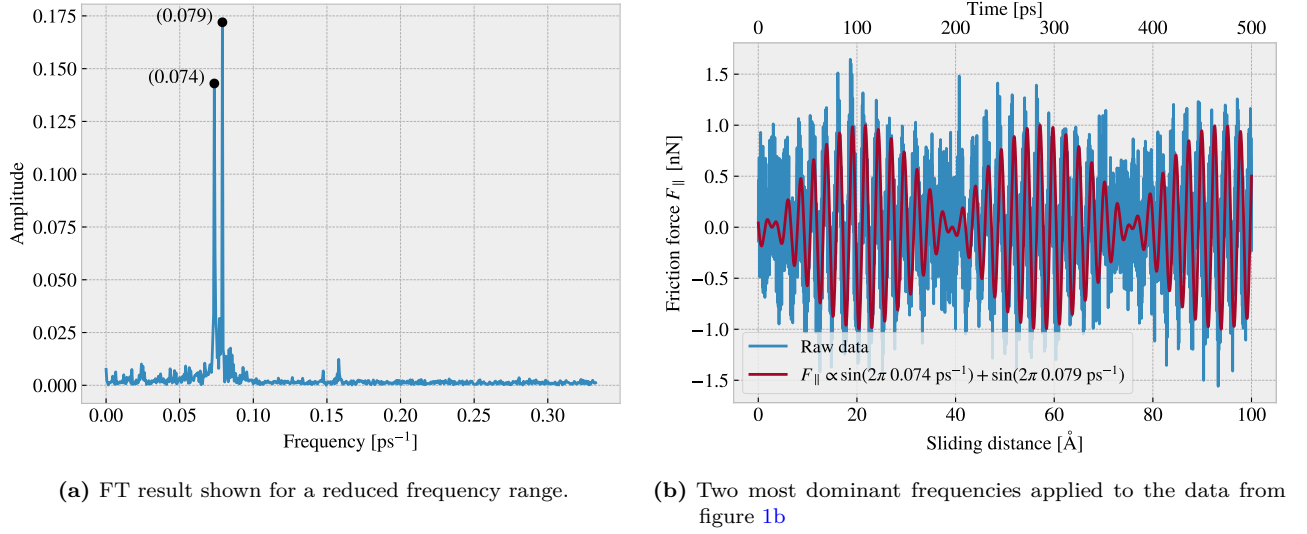
and decomposing  $f_1 = a - b$ ,  $f_2 = a + b$  we can rewrite the sine sum as the sinusoidal product

$$\begin{aligned}\sin(2\pi f_1) \sin(2\pi f_2) &= \sin(2\pi(a - b)) \sin(2\pi(a + b)) \\ &= \sin(a) \cos(b) + \cos(2\pi a) \sin(2\pi b) + \sin(2\pi a) \cos(2\pi b) - \cos(2\pi a) \sin(2\pi b) \\ &= 2 \sin(2\pi a) \cos(2\pi b),\end{aligned}$$

with

$$\begin{aligned}a &= \frac{f_1 + f_2}{2} = 0.0763 \pm 0.0005 \text{ ps}^{-1}, & b &= \frac{f_2 - f_1}{2} = 0.0028 \pm 0.0005 \text{ ps}^{-1}, \\ &= 0.381 \pm 0.003 \text{ \AA}^{-1}, & &= 0.014 \pm 0.003 \text{ \AA}^{-1},\end{aligned}$$

where the latter frequency is denoted with respect to the sliding distance. This makes us recognize the high oscillation frequency as  $a$  and the low frequency as  $b$ . The faster one has a period of  $T_a = 2.62 \pm 0.02 \text{ \AA}^2$ . This corresponds well with the magnitude of the lattice spacing and especially that of graphene at  $2.46 \text{ \AA}$  as expected theoretically (make reference to theory section?). We also take note of the longest period  $T_b = 71 \pm 15 \text{ \AA}^{-1}$  which will be relevant for the evaluation of measurement uncertainty in section 0.6.3.



**Figure 2:** Fourier transform (FT) analysis of the full friction force data (all  $400 \text{ \AA}$  sliding distance) shown in figure 1. (a) shows the two most dominant frequency peaks. Note that no significant peaks was found in a higher frequency than included here. (b) shows a comparison between the raw data and the wavefunction corresponding to the two peaks in figure (a).

### 0.6.2.2 Decompositions

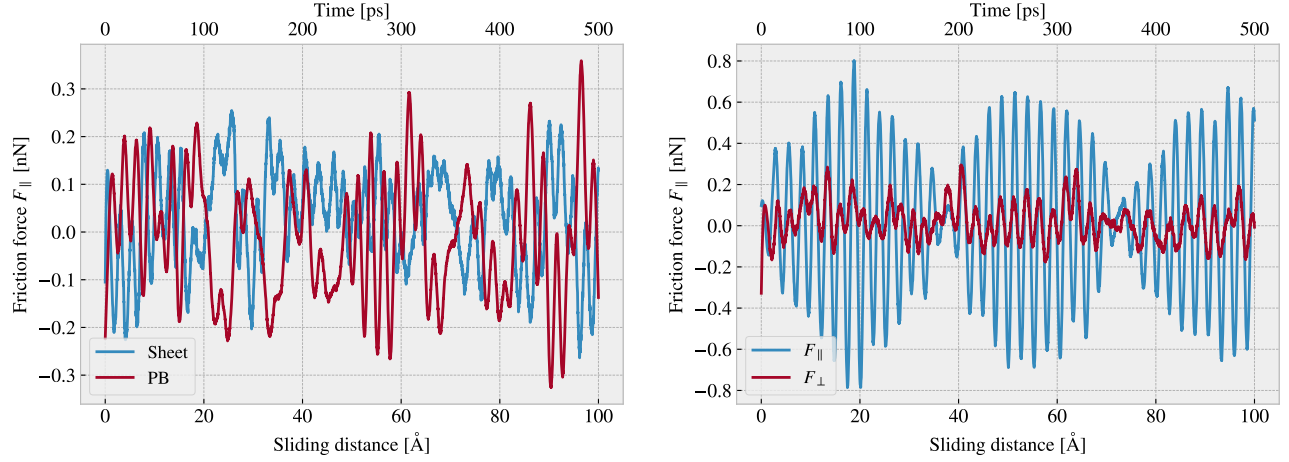
In the previous analysis we have looked only at the friction force for the full sheet, including the pull blocks which is locked off during sliding, and with respect to the drag direction. This represents our choice measurement which we will address in the following.

Due to the fact that we are only applying cuts to the inner sheet (excluding the pull blocks), it might seem more natural to only consider the friction on that part. If the desired frictional properties can be achieved by altering the inner sheet one can argue that any opposing effects from the pull blocks can be mitigated by scaling the relative size between the inner sheet and the pull blocks. However, when looking at the time series of the friction force decomposed with respect to the inner sheet and pull block region (see figure 3a), we observe the friction force arising from those parts are seemingly antisymmetric. That is, the distribution of the frictional pull from the substrate on the sheet is oscillating between the inner sheet and the pull block. Keeping in mind that normal force is only applied to the pull blocks we might take this as an integrated feature of the system which does not necessarily disappear when changing the spatial ratio between inner sheet and pull block. Any interesting friction properties might depend on this internal distribution of forces. Hence, we hedge our bets and use the full sheet friction force as a holistic approach to this measurement problem.

Similar we might question the decision of only considering the frictional force projected onto the sliding direction as we are neglecting the “side shift” induced during the slide phase. In figure 3b we see the decomposition into force components parallel  $F_{\parallel}$  and perpendicular  $F_{\perp}$  to the slide direction respectively. We see that the most dominant trends is projected into the parallel component. If we want to include the perpendicular component as well we would have to evaluate the friction as the length of the force vector for which we would lose the sign of the force direction. Hence, we would only get a positive contribution which would not be able to capture the change between resisting and assisting the sliding during stick-slip motion. One option to accommodate this is by using the vector length but keeping the sign from the projection parallel to the sliding direction. However, we

<sup>2</sup>The uncertainty  $\Delta y$  is calculated as  $\Delta y = \left| \frac{\partial y}{\partial x} \Delta x \right|$  for uncertainty  $\Delta x$  and  $y(x)$

omit such compromises as this might make analysis interpretation more difficult, and we use only the parallel component going forward.

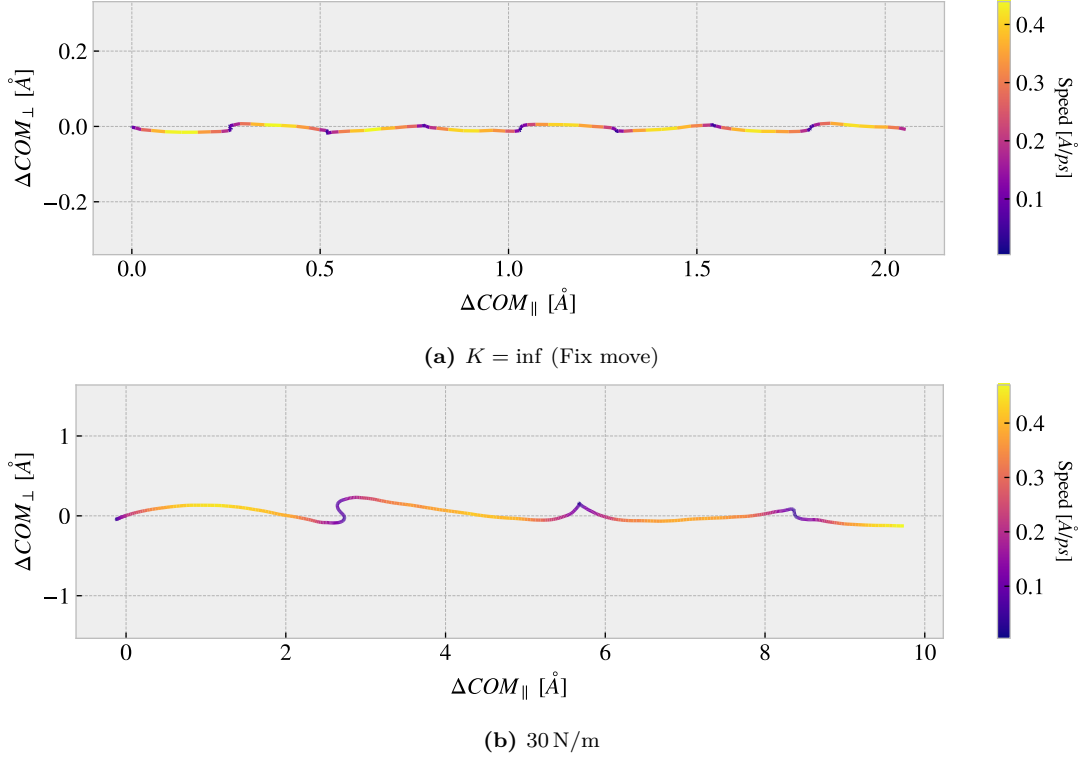


(a) Decomposition into group inner sheet (sheet) and pull blocks (PB). (b) Decomposition into parallel ( $F_{\parallel}$ ) and perpendicular ( $F_{\perp}$ ) to drag sliding direction.

**Figure 3:** Friction force decomposition on the data shown in figure 1 with applied savgol filters similar to that of figure 1b with window polyorder 5 and window length of 150 timesteps (corresponding to a sliding distance of 3 Å or a time window of 15 ps).

### 0.6.2.3 Center of mass path

From the previous observations of the friction force time series we see evidence of a stick-slip behaviour. Specially, we see in figure 3b that this might be the case both parallel and perpendicular to the sliding direction. By looking at the  $x, y$ -position for the sheet center of mass (COM) we observe the stick-slip motion manifested as a variation in COM speed combined with a side to side motion as shown in figure 4a. In an attempt to increase the magnitude of the slips we evaluate a similar simulation with spring constant  $K = 30$  N/m (see figure 4b) in contrast to that of an infinite spring constant. While the maximum slip speed stays within a similar order of magnitude the slip length in the sliding direction is increased along with the side to side motion. Note that the axis scale is different between figure 4a and 4b. However, in both cases we observe that the side to side motion is associated with a low speed, meaning that is more reminiscent of a “slow” creep alignment with the substrate than a slip.



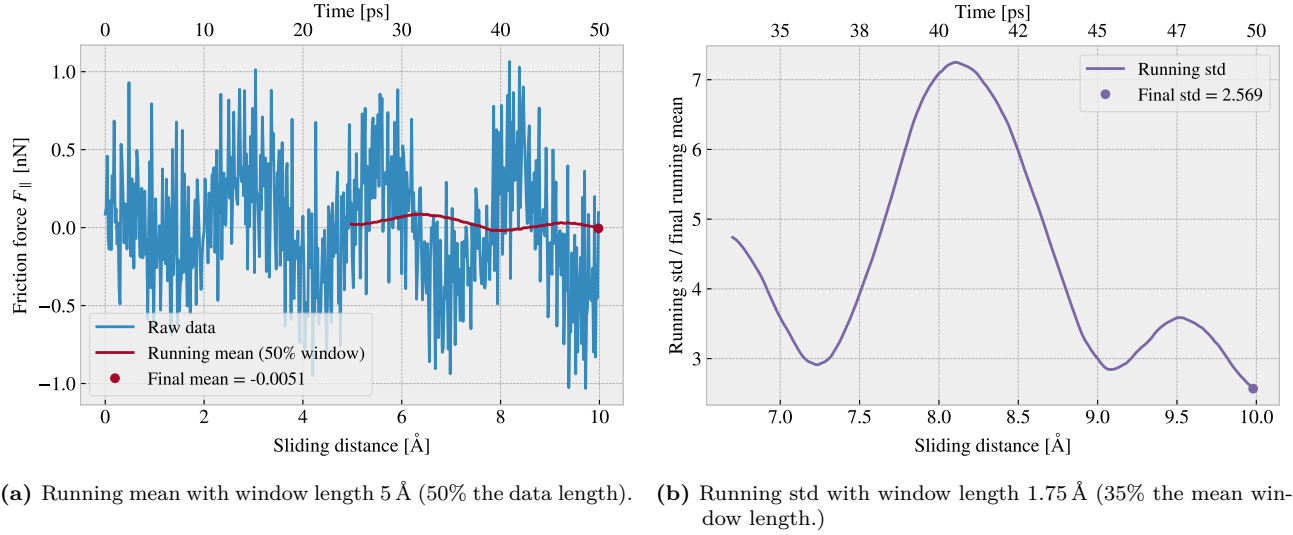
**Figure 4:** Center of mass position relative to the start of the sliding phase in terms of the direction parallel to the sliding direction  $\Delta COM_{\parallel}$  and the axis perpendicular to the sliding direction  $\Delta COM_{\perp}$ . The colorbar denotes the absolute speed of the COM.

### 0.6.3 Defining metrics for dynamic and static friction

In order to evaluate the frictional properties of the sheet we reduce the comprehensive friction force time series addressed in section 0.6.2 into single metrics describing the dynamic and static friction. The natural choice is to use the mean and max values of the time series.

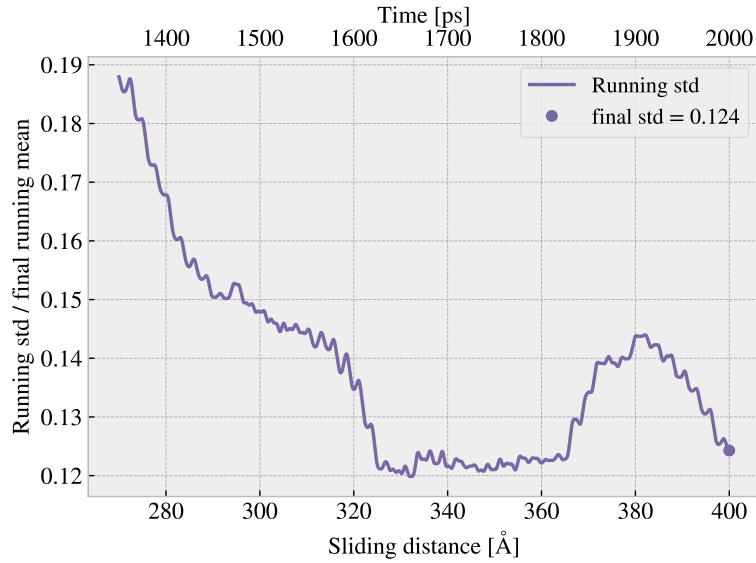
#### 0.6.3.1 Dynamic friction

For the dynamic friction measurement we take the mean value of the latter half of the dataset to ensure that we are sample from a stable system. For a full sliding simulation of 400 Å we thus base our mean value on the latter 200 Å of sliding. In figure 5a we have shown the friction force of the first 10 Å of sliding together with a running mean with window length of 5 Å corresponding to 50% the data length. This is merely done to illustrate the sampling procedure and by only using a 10 Å sliding distance the final mean estimate (indicated with a dot) takes a negative value due to the specific cut-off of the few oscillation captured here. Nonetheless, one approach to quantify the uncertainty of the final mean estimate is to consider the variation of the running mean preceding the final mean value. The more the running mean fluctuates the more uncertainty associated with the final estimate. However, only the running mean “close” to the ending should be considered, since the first part will rely on data from the beginning of the simulation. From the Fourier analyse in section 0.6.2.1 we found the longest significant oscillation period to be  $\sim 71 \text{ Å}^{-1}$  corresponding to  $\sim 35\%$  of the running mean window consisting of 200 Å of sliding when including all the data. Hence, we use the standard deviation of the final 35% of the running mean to approximate the uncertainty of the final mean value, and we estimate the relative error by dividing the standard deviation by the final mean value. In figure 5b we showcase a running standard deviation of a window length 35% the running mean window in figure 5a for the illustrative case of a total 10 Å slide. The final uncertainty value is marked by a dot, and we see as expected that we get a high relative error of  $\sim 257\%$  which corresponds well with the short sampling period and the mean value taking an unphysical negative value.



**Figure 5:** Running mean and running standard deviation (std) on the friction force data from a 10 Å of sliding simulation. The running mean window is 50% the data length while the running std window is 35% the running mean window length.

When including the full dataset of 400 Å of sliding, such that std window actually matches with the longest period of oscillations expected from the data, we get a final relative error of  $\sim 12\%$  as shown in fig 6. This is arguable just at the limit for an acceptable error, but as we shall see later (Make a reference to fig or sec) this high relative error is mainly connected to the cases of low friction. When changing the simulation parameters, such that the mean friction evaluates to considerable higher values, the relative error drops to the order (put in numbers). One interpretation of this finding is simply that the oscillations in the running mean is somewhat independent of the magnitude of the friction. In that case, the relative error will spike for the low friction cases.

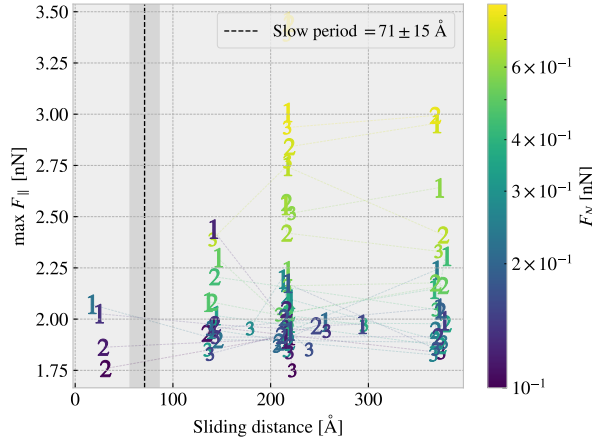


**Figure 6:** Running standard deviation (std) for a full 400 Å sliding simulation. The running std window is 70 Å (35% the running mean window of 50% the data length).

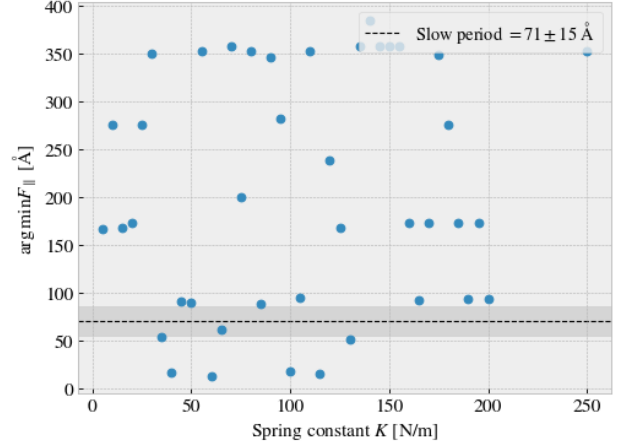
### 0.6.3.2 Static friction

The max value is the most obvious choice for addressing the static friction, even though that the definition of the static friction is a bit vague. When considering the friction force time series in figure 1 we observe that the





**Figure 7:** Distribution of top three max friction force peaks for 30 uniformly sampled normal forces  $F_N \in [0.1, 10]$  nN. The dotted line and the grey area marks the slowest significant oscillation period found in the data and thus marking a dividing line for whether a peak falls within the “beginning” of the sliding simulation.

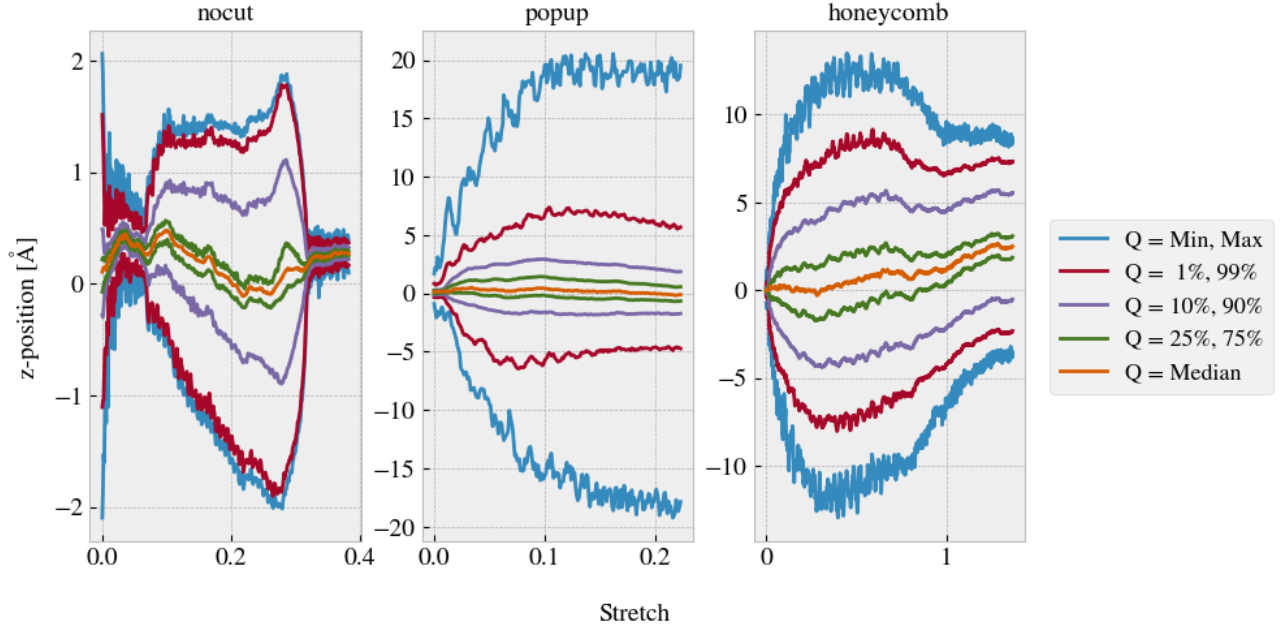


**Figure 8:** Sliding displacement for the max friction peak to appear as a function of spring constant. Fix-move is tmp mapped to  $K = 200$  here without any discontinuous lines.

stick-slip oscillations increase in magnitude toward a global peak at  $\sim 20$  Å. Thus, we could identify this peak as the static friction force, but the global max does in fact rarely fall within the first part of the sliding. In figure 7 we investigate the top three max value, at which sliding distance they occur and at what magnitude, for 30 uniformly sampled normal forces in the interval  $[0.1, 10]$  nN. It is immediately clear that only few of the peaks fall within the “beginning” of the simulation defined by the slowest significant oscillation period of  $71 \pm 15$  Å. In fact only 2/30 global values and 4/90 top three values can be associated to the start of the sliding by this definition. Thus, this result suggests that the max value cannot be used as a reliable measure for the static friction either due to its lack of presence or due to the simulation setup procedure. For a more typical evaluation of the static friction force one would increase force slowly until the first slip significant slip is recorded (a series of precursors is expected to precede this). In our simulations we drag the sheet relatively fast in a rigid manner which made remove... the static friction phenomena. Find reference stating that static friction might disappear when increasing the spring constant of the probe to stiff. By changing the spring constant we investigate possibility to observe a static friction response within the framework of our simulation procedure as shown in figure 8. However, the results do not indicate any implications that a recognizable domain exist for which the static friction response would be reliable. Hence, we will base the final assessment on frictional properties purely on the dynamic friction force.

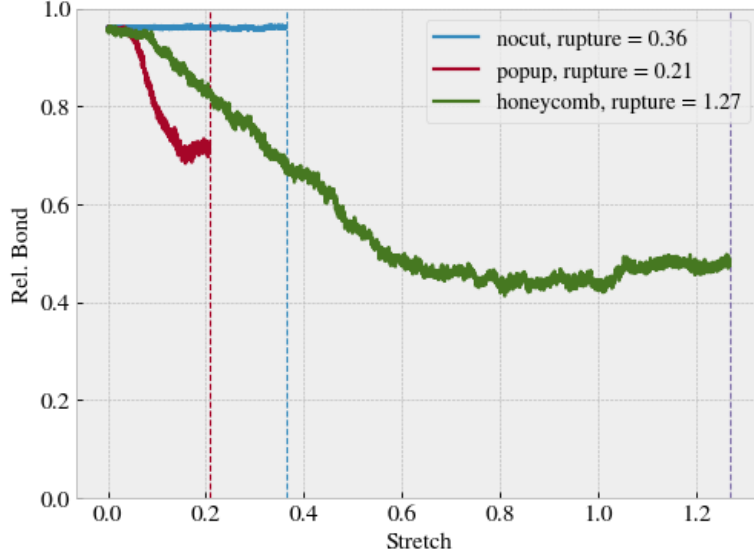
#### 0.6.4 Out of plane buckling

The out of plane buckling is the main motivation for applying the kirigami inspired cuts to the sheet. Thus, we perform a stretch simulation in a low temperature  $T = 5$  K vacuum in order to verify that the chosen cut configurations do in fact contribute to a significant out of plane buckling when stretched. For the non-cut, popup and honeycomb configuration we assess the movement in the z-direction (perpendicular to the plane) during the stretch, which we visualize by the min and max z-value along with the atom count quartiles 1%, 10%, 25%, 50% (median), 75%, 90% and 99% as shown in figure 9. We observe that the popup and honeycomb pattern buckles considerable out of plane during the stretch in comparison to the non-cut sheet which only exhibit minor buckling of  $\sim 2$  Å which is on the same order as the atomic spacing in the sheet. We also notice that the popup pattern buckles more in consideration to the min and max peaks while the 1%, 99% quartiles is on the same magnitude as the honeycomb. By looking at the simulation visualization (include OVITO figures for vacuum stretch as well?) we can conclude that this is mainly due to the fringes of the sheet “flapping” around.



**Figure 9:** Out of plane buckling during stretch of sheets in vacuum at  $T = 5$  K. Reading from left to right the vacuum rupture stretch are 0.38, 0.22 and 1.37. [perhaps use a color scale instead of the standard color cycles here.](#)

The next step is to verify that the buckling will lead to a significant altering of the contact area when the sheet is in put in contact with the substrate. We investigate this by simulating the stretch at the default temperature  $T = 300$  K with the presence of contact forces between the sheet and substrate. Note that no normal load is applied as the sheet and substrate is sufficiently attracted by the LJ potential. Selected frames from the simulation is shown in appendix ???. We assess the contact area by the relative amount of atoms in the sheet within chemical range of the substrate. The cut-off for this interaction is  $4 \text{ \AA}$  corresponding to  $\sim 120\%$  the LJ equilibrium distance. Since the contact area is usually calculated as the amount of atoms in contact multiplied with an associated area for each contact this feature is taken to be proportional to the contact area. The relative amount of bonds as a function of stretch for the various configurations is shown in figure 10 which clearly indicates a drop in contact area as the cutted sheets are stretched.

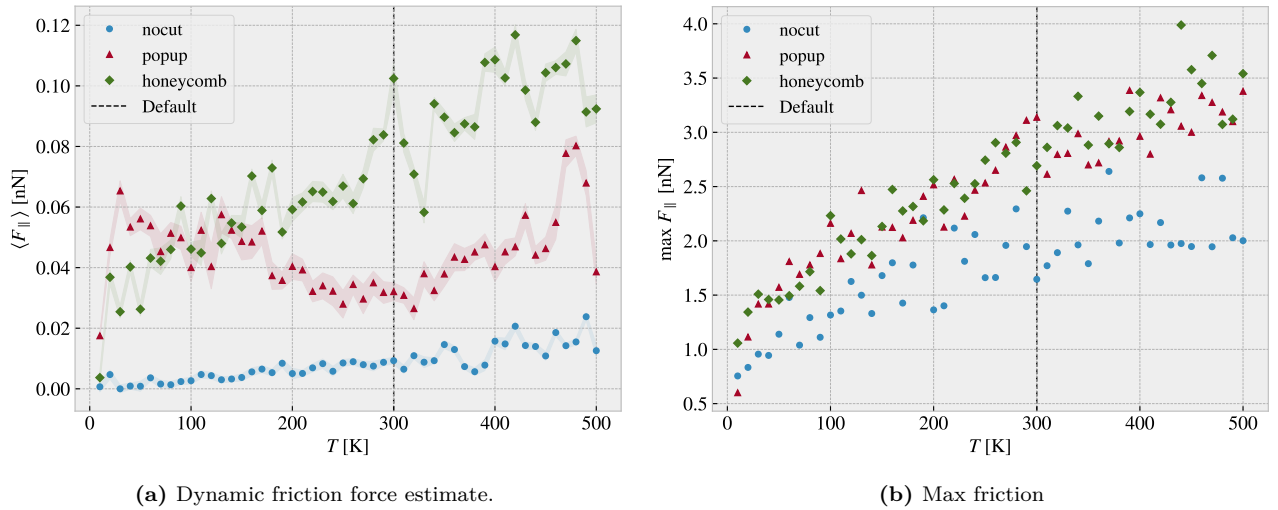


**Figure 10:** Contact vs. stretching of the sheet, where the contact is measured by the relative amount atoms in the sheet within chemical interaction range to the substrate. The cut-off for this interaction range is 4 Å corresponding to  $\sim 120\%$  the LJ equilibrium distance.  $T = 300$  K

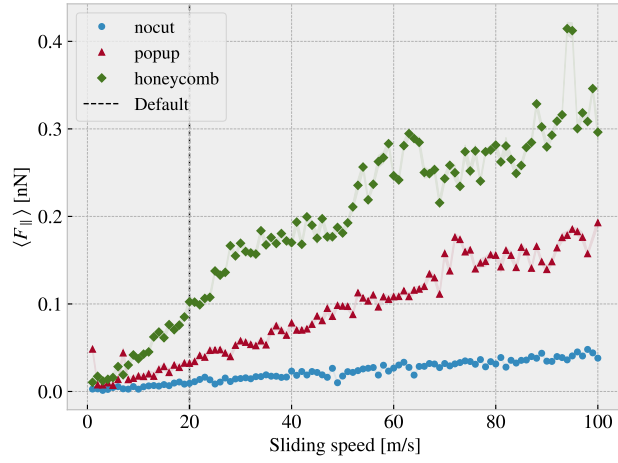
Compare figure 10 to that of figure 15 where multiple simulations constitute the stretch-contact curve.

### 0.6.5 Investigating selected parameters

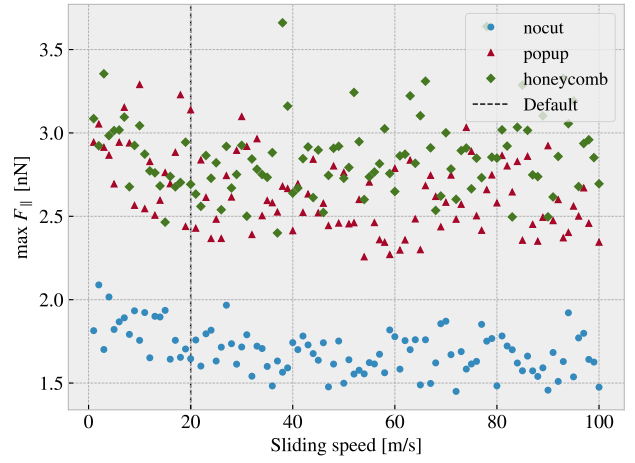
We investigate the importance of the physical variables  $T$ ,  $v_{\text{slide}}$  and  $K$  (make plots for scan angle as well?) and the choice of timestep  $dt$ . This is done partly to understand how the dependencies relate to theoretical, numerical and experimental results, and partly to understand how these parameter choices define the regime for our multi configurational search. We use the default parameters in table 2 with exception of the single parameter of interest which is varied in a reasonable range of the default choice. In figure 11-14 the dynamic friction estimate and the max friction force is shown as a function of  $T$ ,  $v_{\text{slide}}$ ,  $K$  and  $dt$  respectively. For the dynamic friction estimate the absolute error is denoted by a shaded error which linearly connects the points.



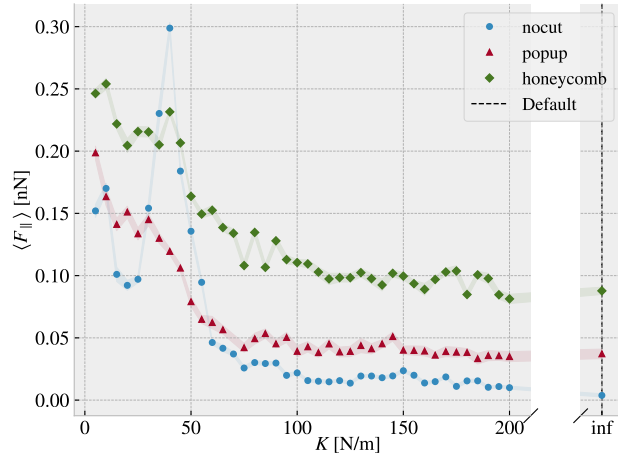
**Figure 11:** Temperature.



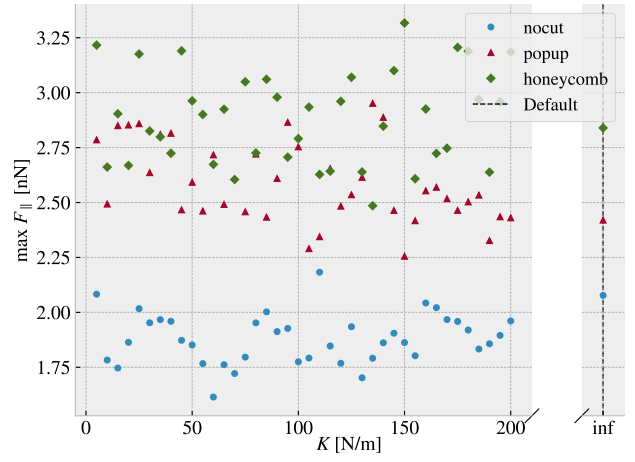
(a) Dynamic friction force estimate.



(b) Max friction

**Figure 12:** Sliding speed

(a) Dynamic friction force estimate.



(b) Max friction

**Figure 13:** Spring constant

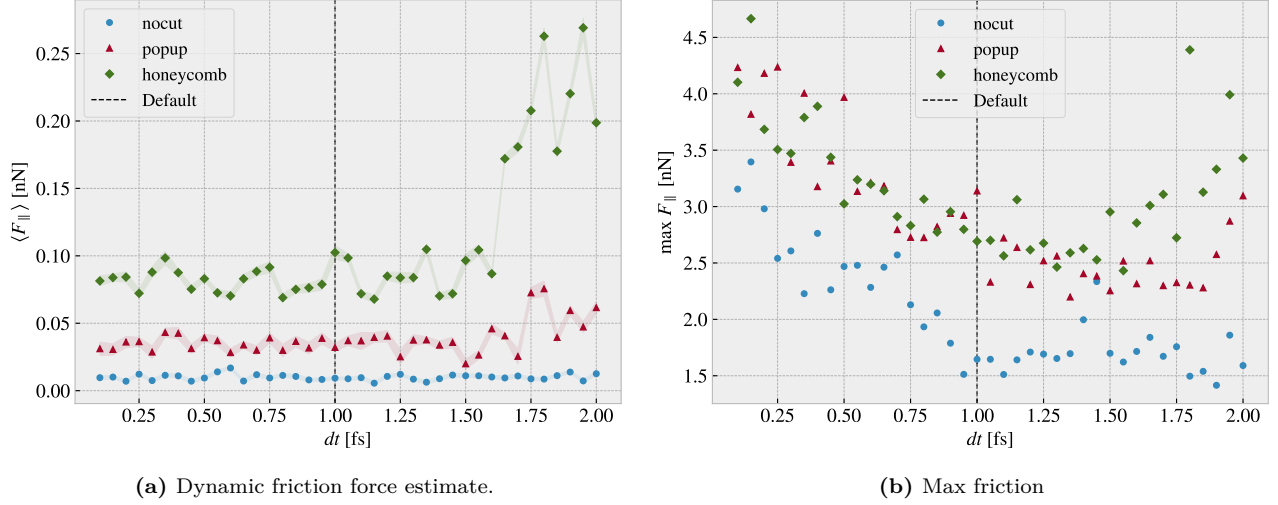


Figure 14: Timestep

Quick thoughts:

- Temperature: We do clearly not see the  $1/T$  temperature decrease. The non cut sheet seems to showcase a linear relationship which is also somewhat present for the honeycomb. For the popup we do see a local decrease at low temperatures which flip at around the default  $T = 300$  K temperature. The max friction peaks seem to increase with temperature as well indicating that the peaks might be associated with thermal fluctuations rather than actual stick-slip behaviour. This supports the finding that the static friction response is not significantly present in these simulations.
- Velocity: Considering the non-cut sheet first the velocity dependency is seemingly linear which deviates from the expected logarithmic trend. For the cutted configurations we find some peaks which might indicate the presence of resonance frequencies. The cutted sheet might be closer to a logarithmic trend, but this is not spot on either. The max friction seems to decrease slightly with small velocities and then stay rather constant. This can probably be explained by the reduced time to stick between stick slip.
- Spring constant: On all three configurations the dynamic friction decreases with an increasing spring constant. The best explanations might be due to the lack of freedom to “get stuck” in incommensurable configurations. We also notice that the friction varies a lot at lower spring constants supporting the choice of having a stiff spring for stability reasons. Especially the non-cut sheet peaks at  $K = 40$  N/m. The max friction seem to be constant with  $K$ .
- $dt$ : The dynamic friction is relatively stable around the default choice of  $dt = 1$  fs. However, the fluctuations with respect to  $dt$  is more significant for popup pattern and even more for the honeycomb pattern. This indicates that the more complex dynamics of the simulation is more sensitive to the timestep. We might interpret this information as an additional measure of uncertainty. The maximum friction decreases with increasing timestep which can be asserted a statistical interpretation: Higher peaks will be captured by the high resolution of a low  $dt$  and vice versa. The high max values towards the point of  $dt = 2$  fs is most likely due to the approach of instability in the simulation as seen more clearly for the dynamic friction evaluation.

### 0.6.6 Normal force and stretch dependencies

Till this point we have only changed variables one by one to investigate single dependencies. We now advance the study to a simultaneous variation of stretch and normal force.

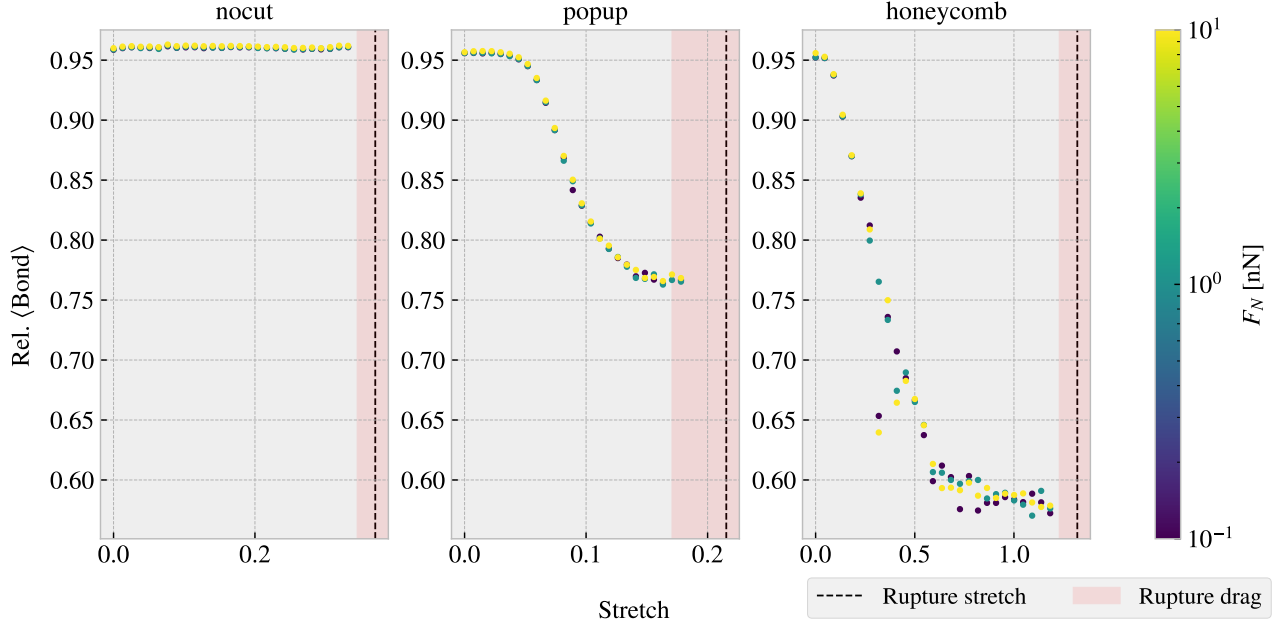
Explain how the stretch is uniformly sampled within equally divided intervals and the normal force is actually uniformly sampled in a given range. Argue that the first might be approximately uniformly distributed for large numbers.

Talk about rupture test also. Maybe in the theory/method section under numerical procedure: Before simulating a rupture test is perform to determine under what stretch the sheet ruptures. This is a slightly higher threshold than when applied normal load and sliding along the substrate.

### 0.6.6.1 Contact area

??

We reproduce the contact area investigation of figure 10 with the modifaciton that the contact count is measured as an average of the latter 50% of the sliding simulation at a non-zero applied normal load. The results are shown in figure 15 with 30 attempted (some rupture) stretch (pseudo) uniformly distributed stretch between 0 and the rupture point and 3 uniform distributed normal loads in the interval  $[0.1, 10]$  nN.

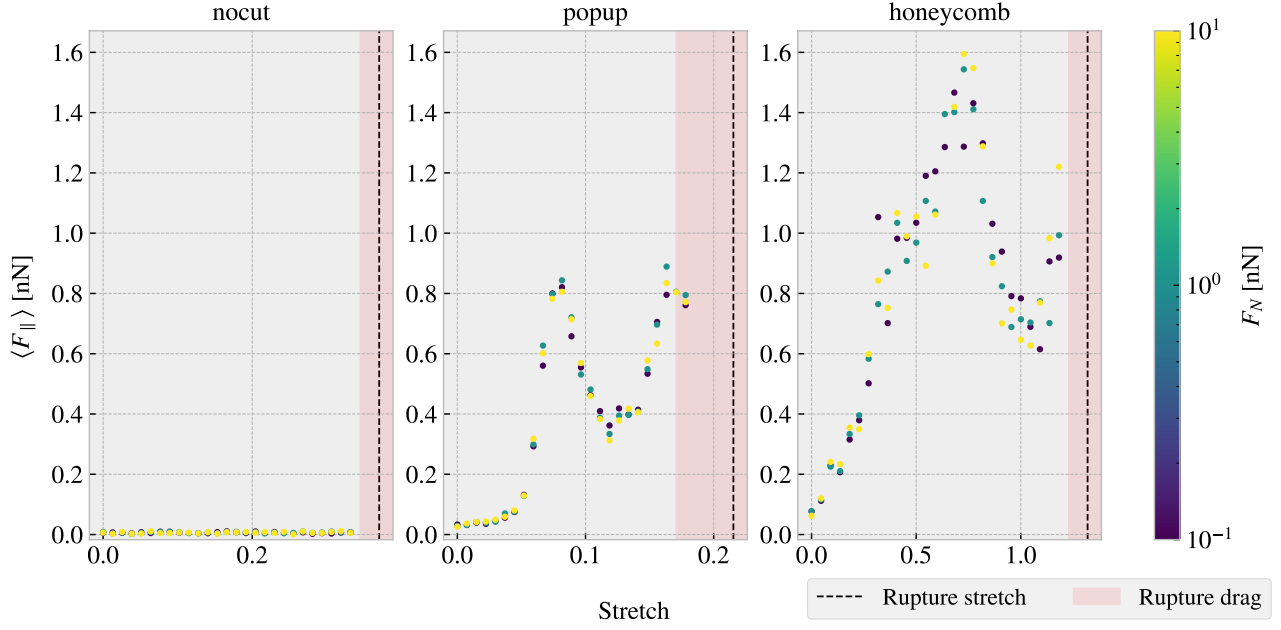


**Figure 15:** Average relative amount of bonds between the sheet and the substrate defined by the cut-off distance of 4 Å. The average is taken over the latter half of the sliding phase. The red shade denotes the stretch range where ruptures occur at certain normal loads under sliding while the black-dotted line represent the rupture point due to stretching (rupture test)

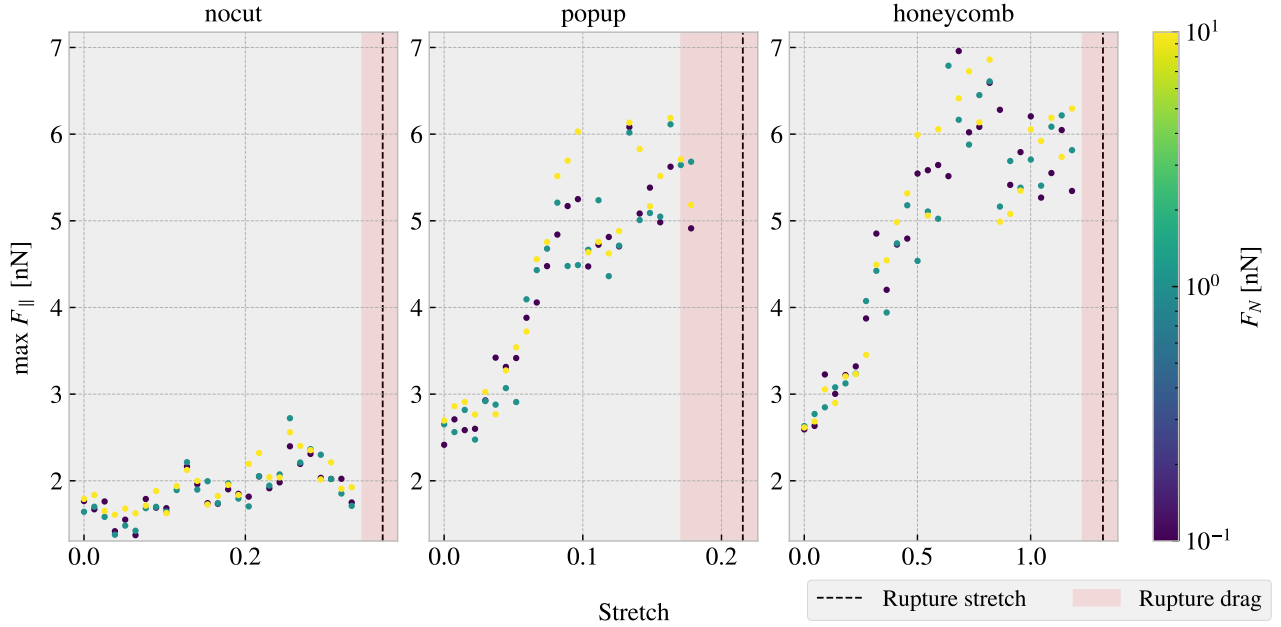
From figure 10 we observe a significant decrease in the contact due to stretching of the cut configurations in contrast to the non-cut which stays roughly constant. This is reminiscent of the non-sliding stretch vs. contact curve shown in figure 10. Given these results, theoretically one would expect the dynamic friction to decrease with stretch for the cut configurations.

### 0.6.6.2 Stretch

We make a similar analysis as done in the previous section ?? with the substitution of friction force instead of contact (The data is taken from the same simulaitons runs). The dynamic friction force (put uncertainty here even though that it is quite low?) and the max friction is shown in figure 16a and 16b respectively.



(a) Dynamic friction estimate.



(b) Max friction

Figure 16: CAPTION

From figure 16a we find to our surprise that the dynamic friction increase with stretch for the cut configurations despite a simultaneous decrease in contact area as shown in figure 15. This suggests that the amount of chemical bonding atoms is not the dominant mechanism for the friction of this system. Instead, we might point to a mechanism more mechanical of nature associated to phonon excitations. When the cut sheet is stretched the stress (show stress maps somewhere or not necessary?) might induce a certain distribution and magnitude of point pressures to favor energy dissipation. Nonetheless, the results showcase a strong coupling between stretch and friction force, also for the max friction force, which is beyond the expectations at this stage of the study. The non-cut configuration does not show significant dependency on the stretch which reveal that this effect is only present when combining cut and stretch and not purely by stretching the sheet.

By considering the increase in dynamic friction towards the first peak we get a relative friction increase and increase vs. stretch ratios as described in table 3. While the honeycomb force increase towards the first peak is approximately linear the popup exhibits seemingly exponential growth which yield a slope on the order  $\sim 30$  nN.

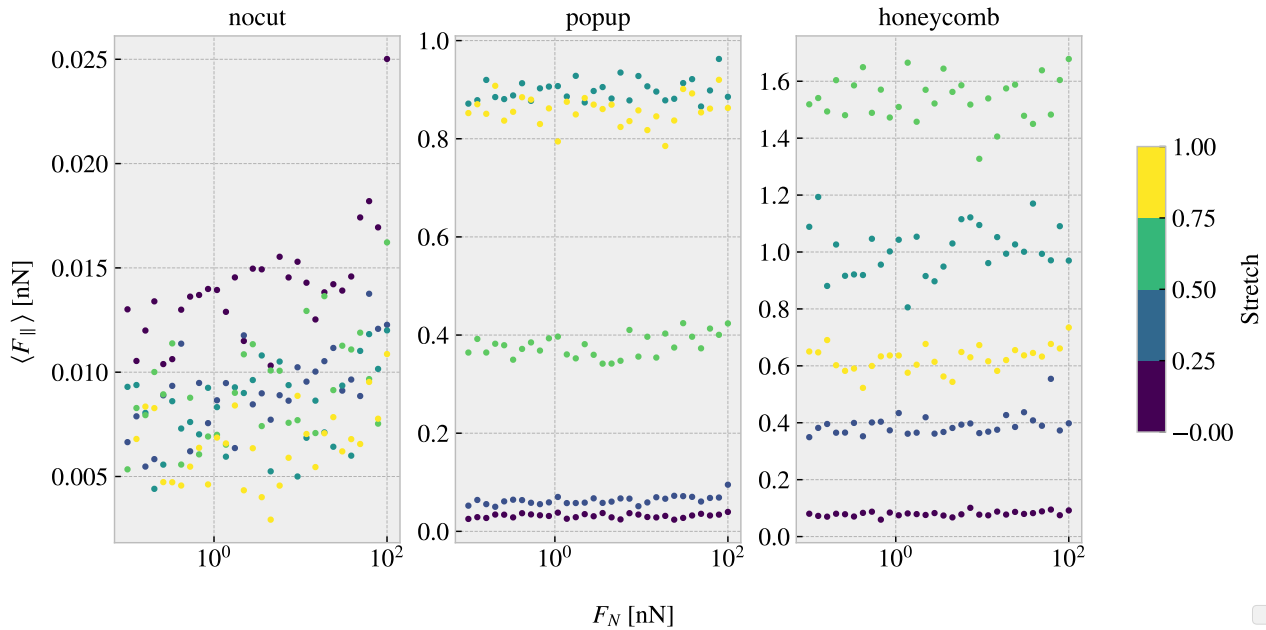
**Table 3:** (stretch, dynamic friction) coordinates from figure 16a at start and the first peak respectively used to approximate the relative increase in friction force and the ratio for friction increase vs. stretch for said range. In practice the latter ratio denotes the slope of a forced linear trend.

Configuration	Start	First peak	Relative increase	Friction force vs. stretch ratio [nN]
Popup	$\sim (0, 0.03)$	$\sim (0.082, 0.83)$	27.7	9.76
Honeycomb	$\sim (0, 0.07)$	$\sim (0.728, 1.57)$	22.4	2.06

Additionally, we notice that both the popup and honeycomb also exhibits stretch ranges where the dynamic friction force decrease with increasing stretch. Qualitatively we assign the slope to be on the same order of magnitude as those towards the first peak. This is useful for the prospect of taking advantage of this phenomenon as we can essentially achieve both higher and lower friction for increasing stretch for different starting points.

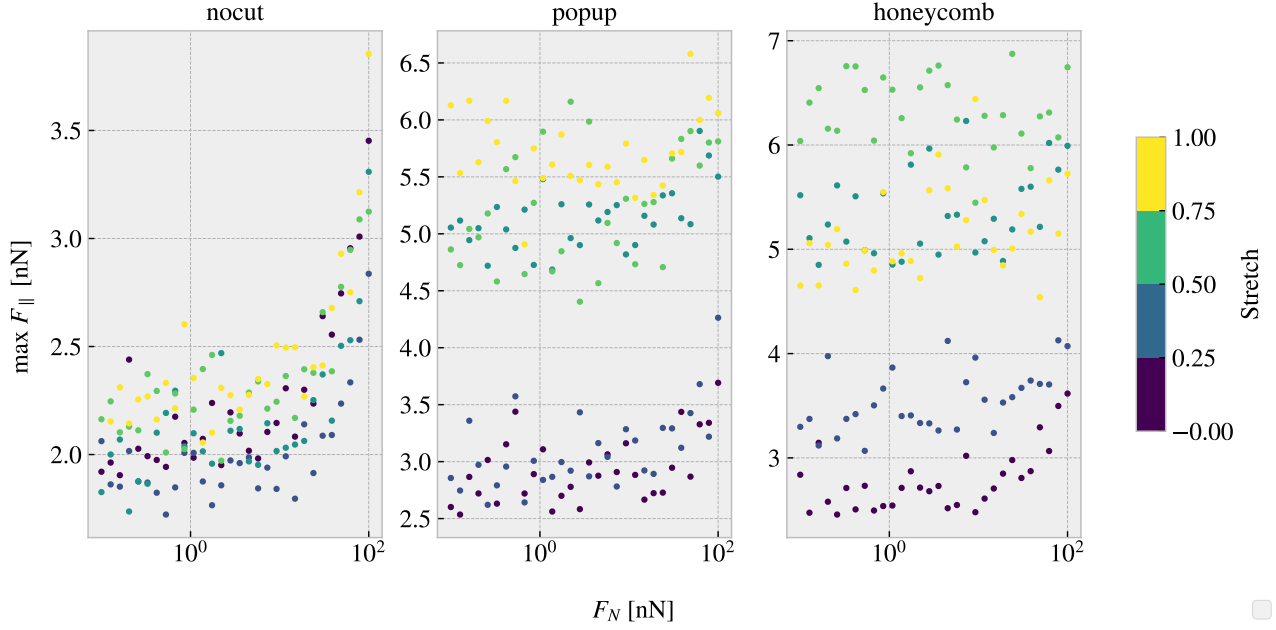
### 0.6.6.3 Normal force

Main take away from this section should be that the normal force does not really change the friction much; The friction coefficient is extremely low, but I'm not sure how well the linear fits are (whether they are linear or sublinear). Not sure if I should do a linearly increasing normal force for better linear plots?



**Figure 17:** ...





**Figure 18:** Colorbar is only fitted for the right plot (honeycomb)... this should be fixed. Should I have run a linear distribution of FN so I could plot it linear here also...?

**Table 4:** Mean friction coeff

nocut	$0.00009 \pm 1 \times 10^{-5}$	$0.00005 \pm 1 \times 10^{-5}$	$0.00004 \pm 1 \times 10^{-5}$	$0.00005 \pm 2 \times 10^{-5}$	
popup	$0.00005 \pm 3 \times 10^{-5}$	$0.00024 \pm 5 \times 10^{-5}$	$0.0002 \pm 2 \times 10^{-4}$	$0.0005 \pm 1 \times 10^{-4}$	$0.0003 \pm 2 \times 10^{-4}$
honeycomb	$0.00013 \pm 6 \times 10^{-5}$	$0.0006 \pm 3 \times 10^{-4}$	$0.0004 \pm 6 \times 10^{-4}$	$0.0007 \pm 6 \times 10^{-4}$	$0.0009 \pm 3 \times 10^{-4}$

**Table 5:** Max fricition coeff

nocut	$0.0139 \pm 9 \times 10^{-4}$	$0.0083 \pm 7 \times 10^{-4}$	$0.010 \pm 1 \times 10^{-3}$	$0.0105 \pm 9 \times 10^{-4}$	
popup	$0.007 \pm 2 \times 10^{-3}$	$0.010 \pm 2 \times 10^{-3}$	$0.007 \pm 2 \times 10^{-3}$	$0.009 \pm 3 \times 10^{-3}$	$0.006 \pm 2 \times 10^{-3}$
honeycomb	$0.010 \pm 1 \times 10^{-3}$	$0.007 \pm 2 \times 10^{-3}$	$0.007 \pm 3 \times 10^{-3}$	$0.000 \pm 3 \times 10^{-3}$	$0.004 \pm 3 \times 10^{-3}$

One theory for the low friction coefficient might dependent on the fact that the normal force is only applied on the pull blocks. Especially with the cutted sheet the tension drops such that the effective normal force on the inner sheet is not changing very much. By this theory the friction force vs. normal force on the pull blocks should look a bit more like expected and we might make some plots of thoose to check

When looking at the graphs for the PB the max friction is visually textbook linear, while the mean friction is a bit more linear but also with negativ coefficients...

### 0.6.7 Computational cost

Talk about the computatonal cost of different choices. How does computation time scale with drag speed,  $dt$  and maybe  $T$  and  $K$  as well. One could also mention scaling with system size.

Show how the number of cores per simulation scale to argue that running on just one core (maybe 4) is smart for the next step of many simulations.

Mention the trouble with GPU to show that this was considered, and in fact this was the reason for choosing the Tersoff potential over the AIREBO which is perhaps more common these days...

## 0.7 Generating data

Present the configuration and variable choices for the generated dataset. Perhaps include appendix with all the configurations shown in a grid

## 0.8 Training forward network

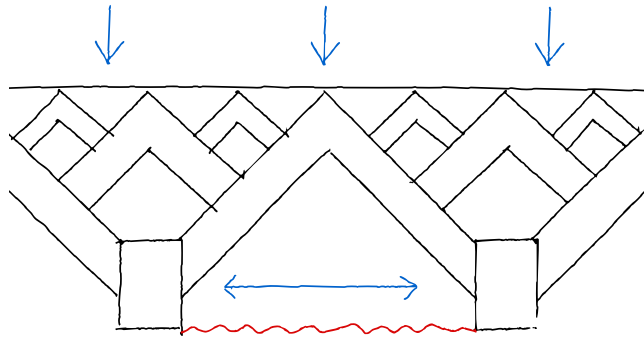
## 0.9 Inverse design

## 0.10 Negative friction coefficient

### 0.10.1 Simulated coupling of normal force and stretch

### 0.10.2 Nanomachine coupling

Attempt to couple normal force and stretch by crossed carbon nanotube (CNT) contraption [19](#).



**Figure 19:** Working sketch for nanomachine

# Appendices



# Appendix A



# Bibliography

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