

Title

Subtitle

by

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THESIS

for the degree of

MASTER OF SCIENCE



Faculty of Mathematics and Natural Sciences
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Title

Subtitle

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Title

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Abstract

Abstract.

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"> - T: Temperature for the Langevin thermostat. - v_{slide} : Sliding speed for the sheet translation. - K: 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). - Scan angle: The direction for which we translate the sheet. 	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"> - dt: Integration timestep. - t_R: Relaxation time before stretching. - Pauses between stretch and adding normal force and between dragging the sheet. - Stretch Speed: How fast to stretch the sheet. - Slide distance: How far to translate the sheet. - Sheet size: Spatial size of the 2D sheet. - Pull block size. 	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"> - Sheet configuration: A binary matrix containing information of which atoms are removed (0) and which are still present (1) in the graphene sheet. - Stretch amount: The relative sheet stretch in percentage. - F_N: Applied normal force to the pull blocks. 	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 way 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 ps^{-1} Slide distance = 400 \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 man¹ 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 cm^2 the pressure drops to a mere 70 kPa corresponding to $\sim 0.01 \text{ nN}$.

¹Yes, 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 \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.

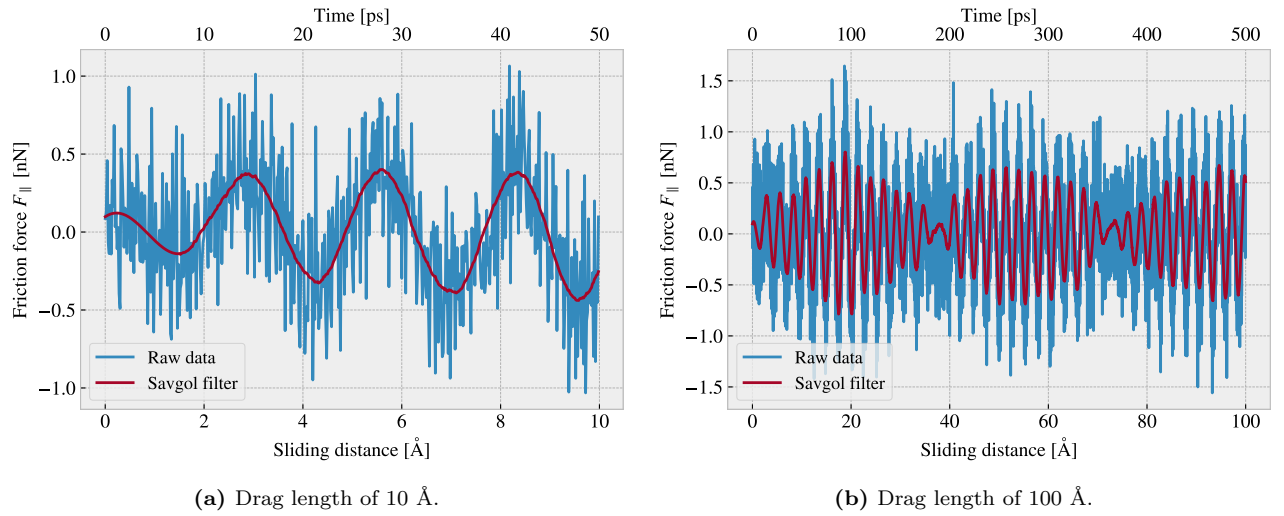


Figure 1: Friction force F_{\parallel} with respect to the drag direction between (full) sheet and substrate versus sliding distance. The sliding distance is measured by the constant movement of the virtual atom and not the COM of the sheet. However, we expect these measures to be fairly identical due 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 \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

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

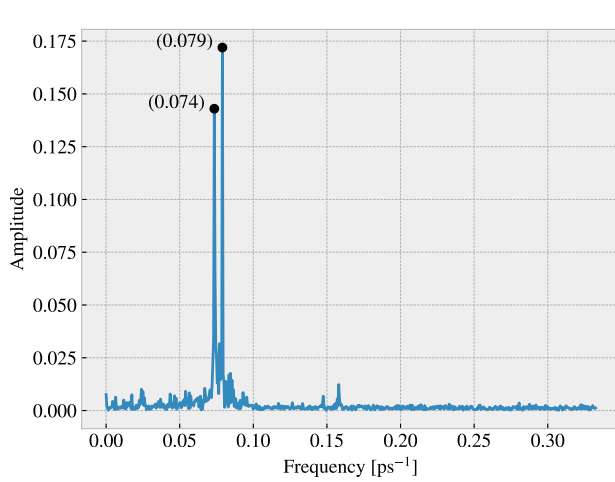
and decomposing $f_1 = a - b$, $f_2 = a + b$ we can rewrite the sine sum as the sinusoidal product

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

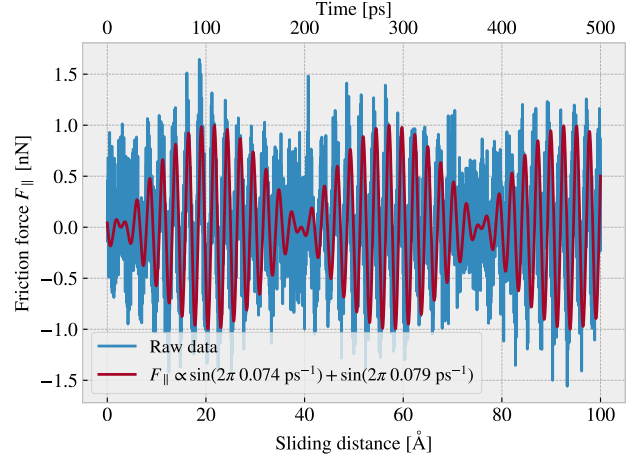
with

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

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 \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.



(a) FT result shown for a reduced frequency range.



(b) Two most dominant frequencies applied to the data from figure 1b

Figure 2: Fourier transform (FT) analysis of the full friction force data (all 400 \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

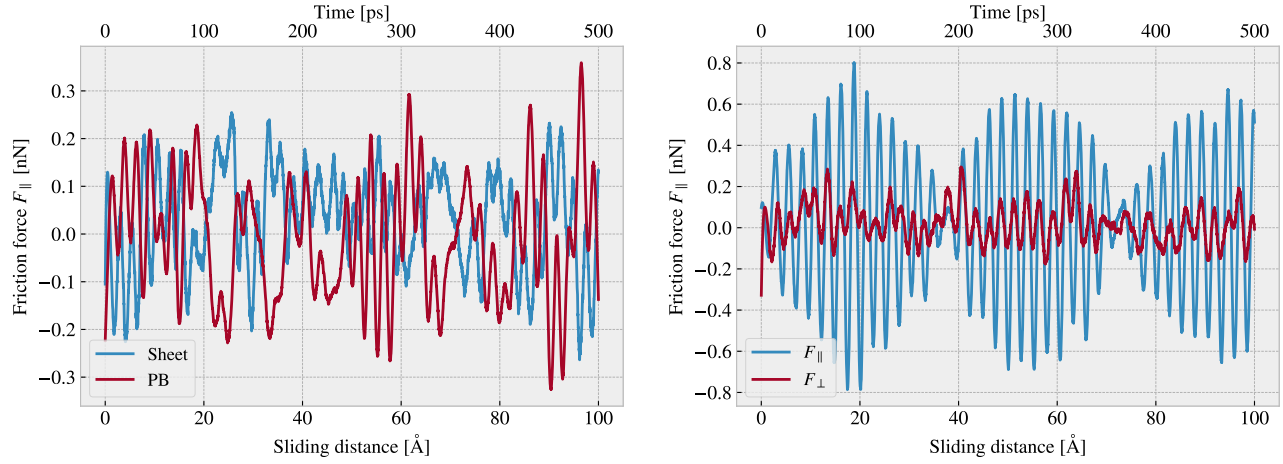
In the previous analysis we have looked only at the friction force for the full sheet, including the pull blocks which is locked off during sliding, and with respect to the drag direction. This represents our choice measurement which we will address in the following.

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

²The uncertainty Δy is calculated as $\Delta y = \left| \frac{\partial y}{\partial x} \Delta x \right|$ for uncertainty Δx 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 we already have evidence of a stick slip behaviour, judging from the friction oscillations in figure 1, and motion partial motion perpendicular to the drag direction, judging from the perpendicular force component in figure 3b. By looking at the x, y -position for the center of mass (COM) we can see the stick slip motion manifested as a variation in COM speed combined with a side to side motion as shown in figure 4a. To increase this effect we also show the same plot with a spring ... move with spring constant 30 N/m in figure 4b. While the max speed is on the same scale the side to side motion is increased (notice that the axis scale is different between figure 4a and 4a).

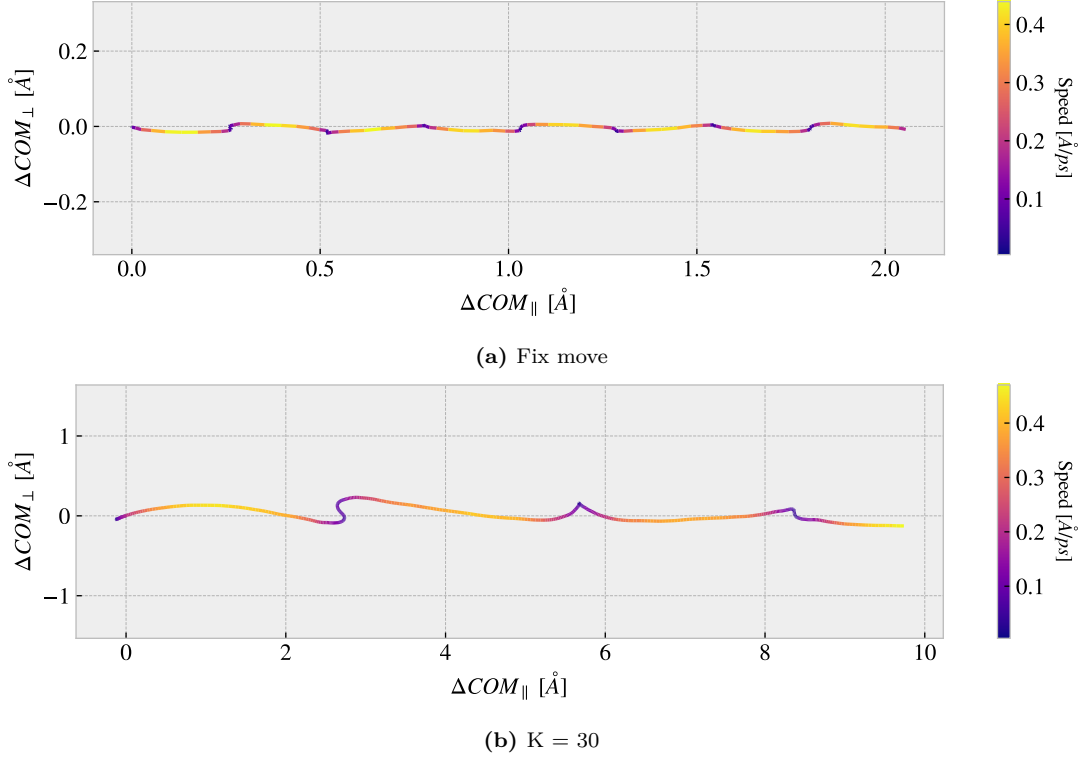


Figure 4: Center of mass relative position from start of drag phase in terms of axis parallel to drag direction ΔCOM_{\parallel} and axis perpendicular to drag direction ΔCOM_{\perp} . The colorbar denotes the absolute speed of the COM.

0.6.3 Defining metrics for dynamic and static friction

We are interested taking the comprehensive friction force time series dataset and reducing it into single metrics describing the dynamic and static friction respectively. The natural choice is to use the mean and max values.

0.6.3.1 Dynamic friction

For the dynamic friction measurement we take the mean of the latter half of the data to ensure that the system has stabilised itself before taking the mean. For a full drag simulation of 400 Å we would thus base our mean value on the latter 200 Å drag. In figure 5a we have shown the friction force of the first 10 Å of drag together with a running mean with window length 50% of the corresponding data length. The final mean value estimate is indicated with red point at the end and we clearly observe that the length of sampling is insufficient since we get a negative friction force. Nonetheless, one approach to quantify the uncertainty of the final mean estimate is to consider the running mean. The more the running mean fluctuates the more uncertainty is associated with the final estimate.

We should not care for fluctuations in the initial part of the running mean curve as this is still including data from the beginning, where it might transition from static to dynamic friction. Only the running mean “close” to the ending should be considered for our uncertainty. From the Fourier analyse we concluded that longest period of any dominant oscillations is $\sim 71 \text{ Å}^{-1}$ corresponding to $\sim 35\%$ of the running mean window of 200 Å drag. Hence we use standard deviation of the final 35% of the running mean curve to approximate the uncertainty of the final mean value. By dividing with the final running mean we effectively calculate the relative error as shown in figure 5b. Naturally, we get a relative error of $\sim 257\%$ which corresponds with the mean value taking an unexpected negative value.

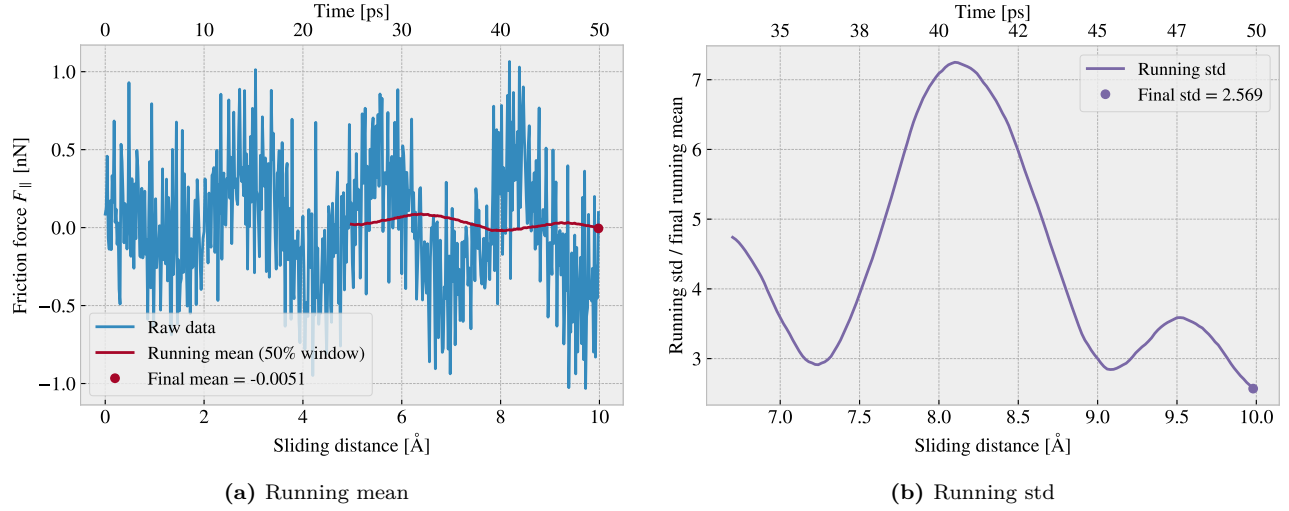


Figure 5: Running std

When we include the full 400 Å drag, 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 just at the limit for an acceptable error, but as we shall see later (refer to figure or something) this high error is mainly connected to the cases of low friction. When changing the simulation parameters, such that the mean friction evaluate to considerable higher values, the relative error drops to around (put in numbers). One explanation is that the oscillations in the running mean does not increase linearly with the magnitude of the friction, and hence the relative error might spike especially for the low friction cases.

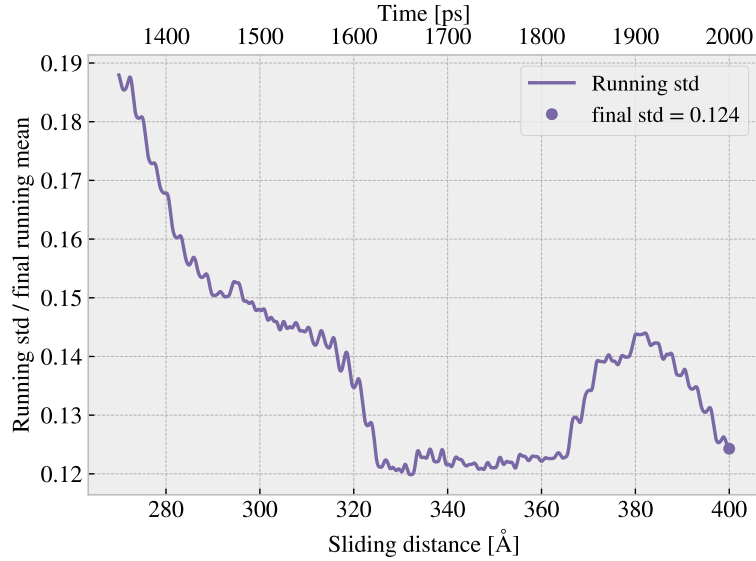


Figure 6: ...

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. At least when judging from the raw data in figure 1 we not see a textbook example of the static friction precursor (maybe include a classic static friction curve in the theory... I'm not completely sure what to expect here). Additionally the global max value does not always lie in the initial part of the simulation.

For a proper static friction evaluation we should increase force slowly and wait for the slip response. Here we

drag quite fast making it difficult to assess the static response.

We investigate the placement of the max values, i.e. the drag length for which we measure the max friction force. We show the placement of the top three max values for different simulations with varying normal force in figure 7. We observe immediately that only a few top three max values is measured within a full slow period of ~ 71 Å. In fact many max values is measured just before the end of the simulation. This indicates that the naive approach of using the overall max value to describe the static friction coefficient might be a too naive approach. Another approach is to use the max value within a single period, but we do not really know if this period will be similar for all cut patterns and thus this might be limiting.

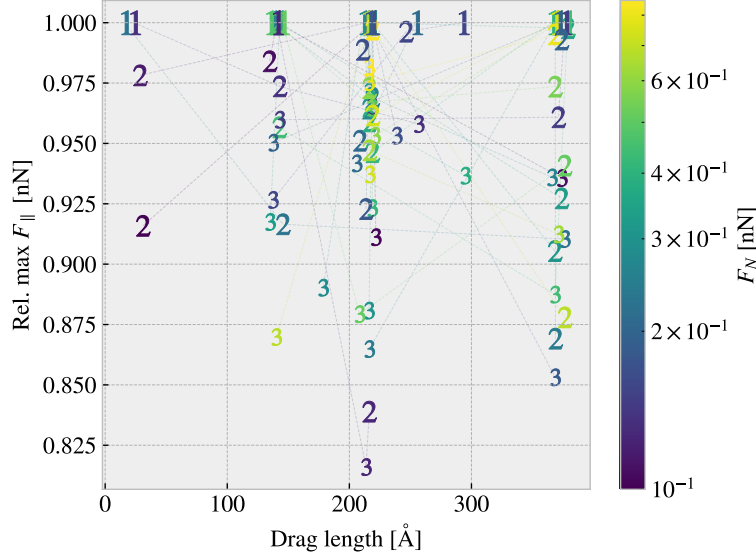


Figure 7: Distribution of top 3 max values for different normal force

Look into static friction when having a spring connected to the drag force with rather low spring constant. Maybe compare to critical stiffness in FK model. Some rough calculations follow here (make a note about this being a very naive approach to determine a suitable stiffness for static friction scenarios. In reality one should increase force slowly to observe this probably). When dragging the sheet in the y-direction we effectively have a lattice spacing

$$a_c = a_{2,x} + B_x = a_G \frac{\sqrt{3}}{2} + \frac{a_G}{2\sqrt{3}} = \frac{2a_G}{\sqrt{3}}$$

for graphene lattice constant $a_G = 2.46$ Å. For the diamond silicon structure this is essentially equal to the lattice constant $a_D = 5.4210$ Å. This gives

$$\theta = \frac{a_c}{a_b} = \frac{2}{\sqrt{3}} \frac{a_G}{a_D} \approx 0.5230.$$

Since we have the factor $2/\sqrt{3}$ it is safe to assume that this is an irrational number leading to incommensurability. The worst case scenario of incommensurability (where θ equals the golden-mean, Can we get the exact number?) gives the minimal critical stiffness $K_c \sim 2U_0(\frac{\pi}{a_b})^2$, where U_0 is the substrate potential magnitude and a_b the lattice spacing of the substrate. The potential barrier U_0 can be approximated by the work done when resisting the normal force as $\sim F_N a_D/2$ such that the critical stiffness can be approximated to

$$K_c \sim 2F_N \frac{a_D}{2} \left(\frac{\pi}{a_D} \right)^2 = \frac{F_N}{a_D} \pi^2$$

With a normal force of 1 nN we get $K_c \sim 18$ N/m. Hence, we should try a spring constant lower than that as qualified way of determining if this is the reason why we do not really see static friction in the simulation. By

plotting the max position (in terms of drag length) as a function of spring constant as seen in figure 8 we can investigate if the concept of a critical spring constant is governing this simulation. However, as I'm writing this I'm realizing that the spring constant in the model applies to the interatomic forces and not the one dragging the system....

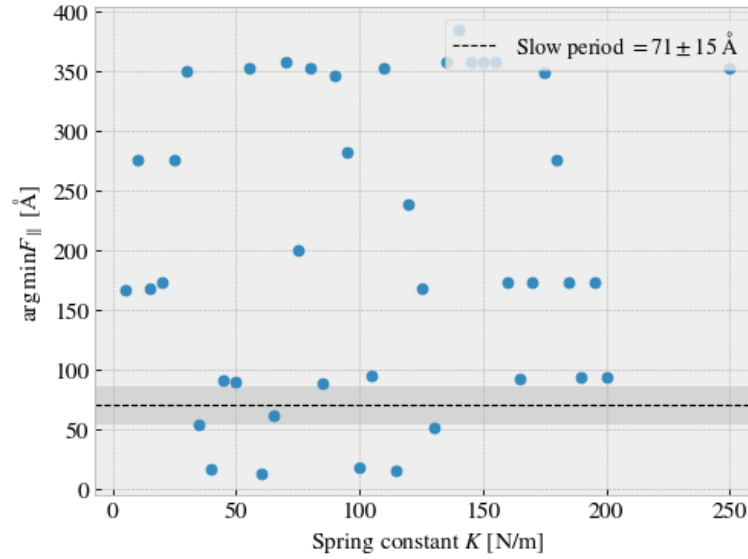


Figure 8: Displacement for the max peak in friction to appear as a function of spring constant dragging the sheet. Fixmove is tmp mapped to $K = 200$ here.

0.6.4 Out of plane buckling

Vacuum test at $T = 5\text{K}$. We see that the popup and honeycomb pattern buckles considerable out of plane during the stretch while the noncut sheet only experiences minor buckling of $\sim 2\text{ \AA}$ which is on the same scale as the atomic spacing in the sheet. We also notice that the popup pattern experiences buckles more in consideration to the min and max peaks while the 1%, 99% quartiles is on the same scale as the honeycomb. By looking at the visualization (include this somewhere) we can conclude that this is mainly due to the fringes of the sheet “flapping” around.

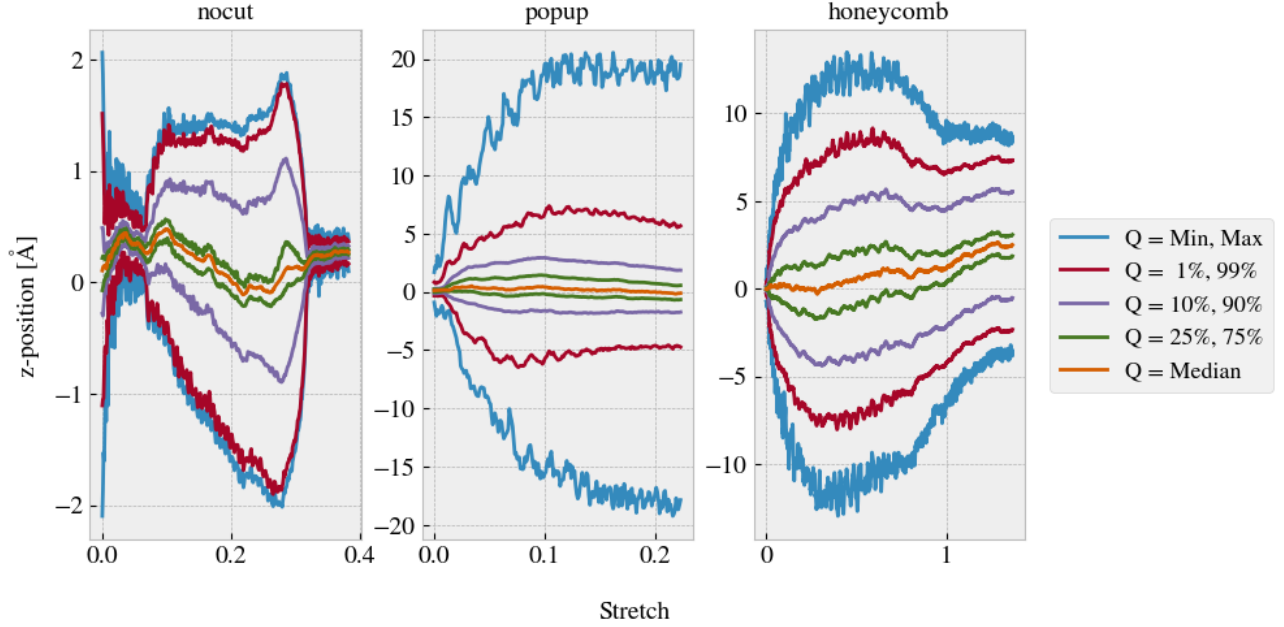


Figure 9: Out of plane buckling during stretch of sheets in vacuum at $T = 5\text{ K}$. Reading from left to right the vacuum rupture stretch are 0.38, 0.22 and 1.37.

Similar test is performed in the presence of the substrate under a higher temperature $T = 300\text{ K}$. 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 \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 proportional to that.

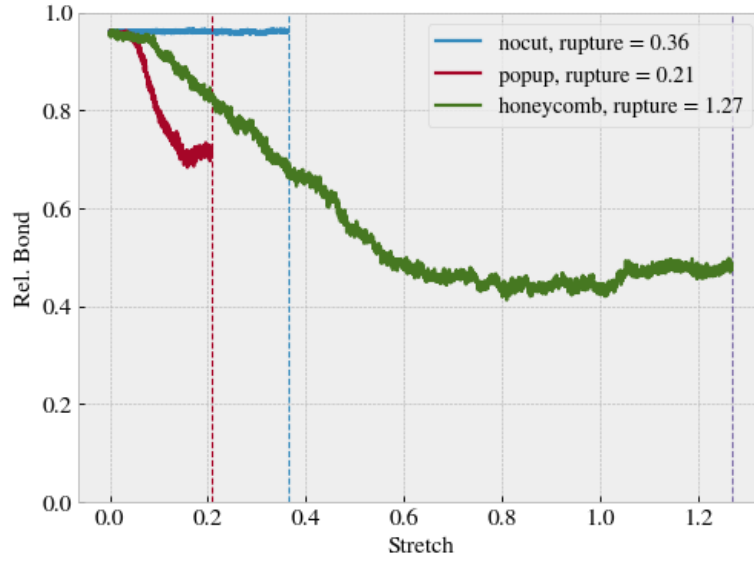


Figure 10: Contact vs. stretching of the sheet, where the contact is measured by the relative amount atoms in the sheet within chemical interaction range to the substrate. The cut-off for this interaction range is 4 \AA corresponding to $\sim 120\%$ the LJ equilibrium distance. $T = 300 \text{ K}$

0.6.5 Investigating selected parameters

Investigate effects of temperature, drag speed, spring constant and dt.

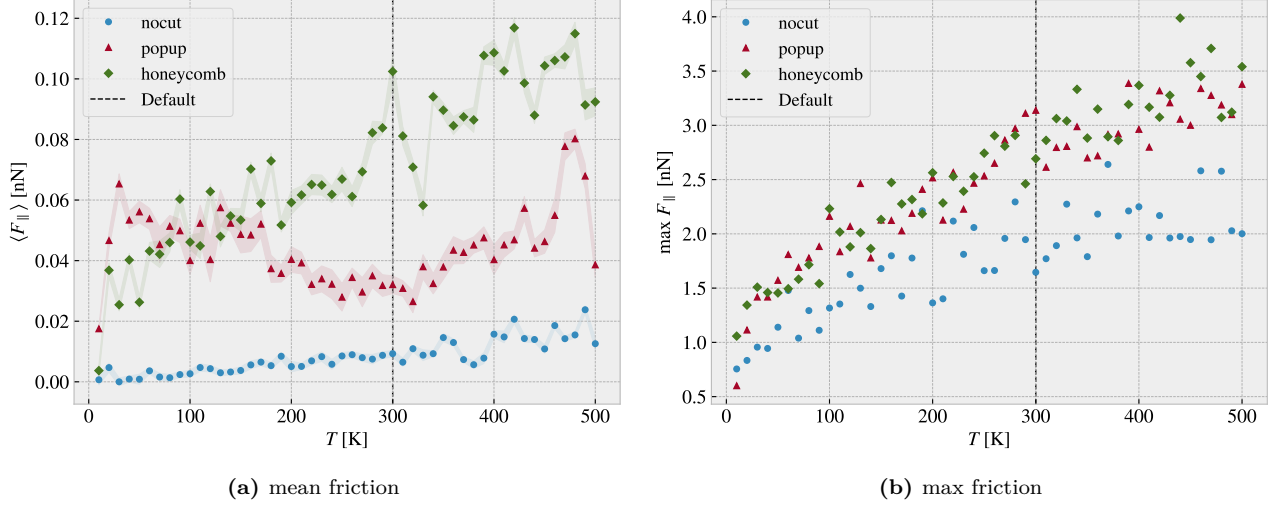


Figure 11: Temperature. $v = 20$ m/s and fixmove.

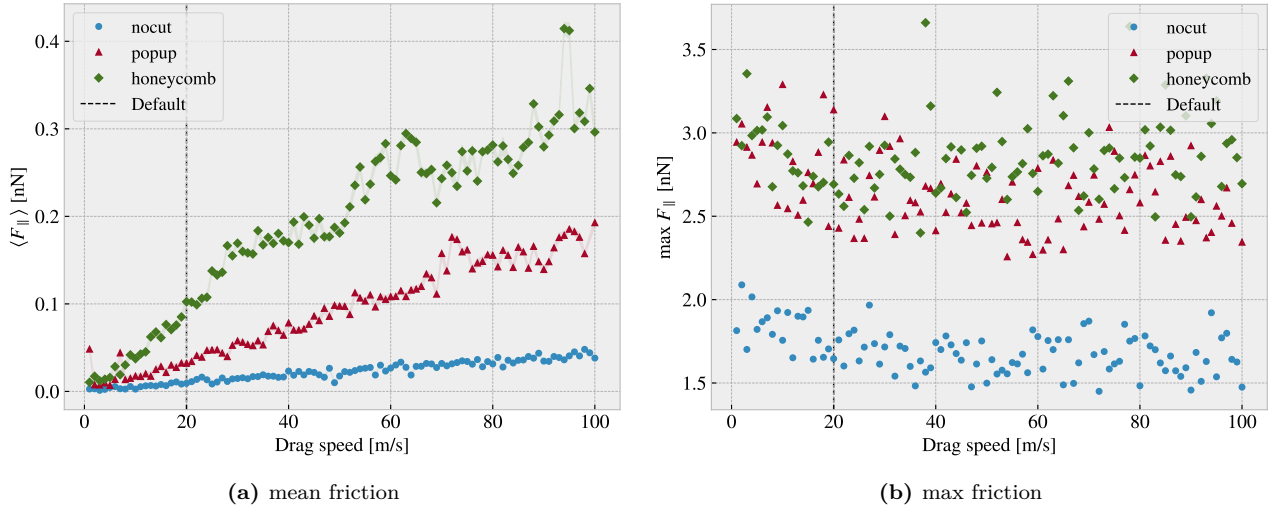
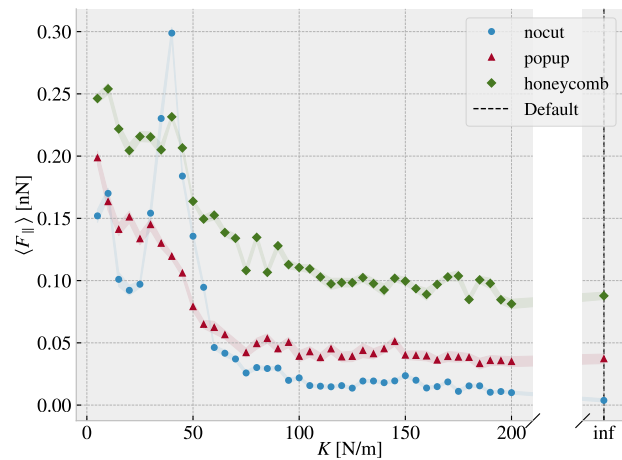
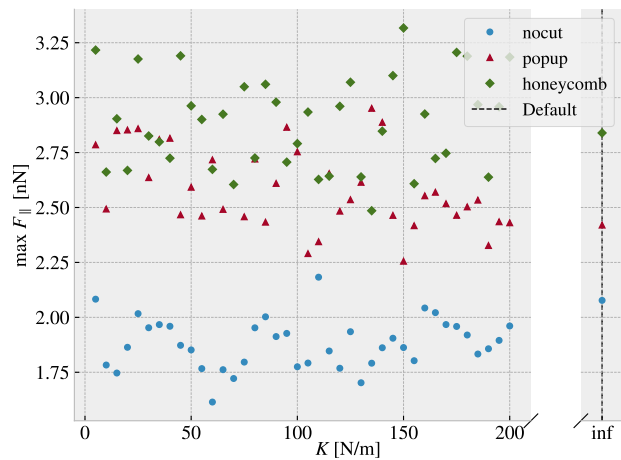


Figure 12: Drag speed

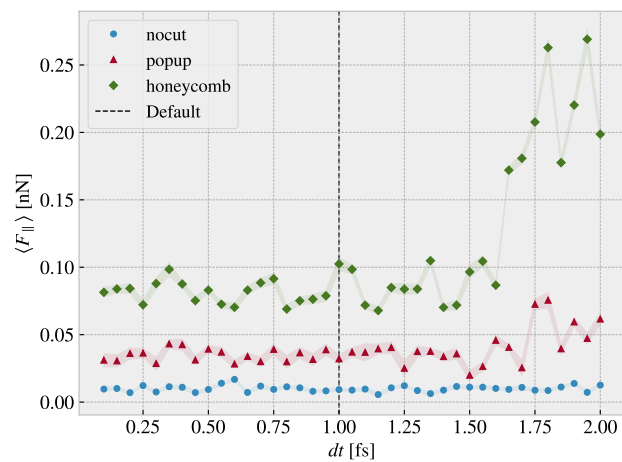
Simulations of concentric nanotubes in relative motion (telescopic sliding), have revealed the occurrence of well-defined velocities at which friction is enhanced, corresponding to a washboard frequency resonating with longitudinal [172] or circular [173] phonon modes, leading to enhanced energy dissipation. The frictional response becomes highly non-linear while approaching the critical velocity and, contrary to macroscopic systems, washboard resonances can arise at multiple velocities, especially for incommensurate interfaces where more than one length scale may be in common to the contacting surfaces [172] [6].



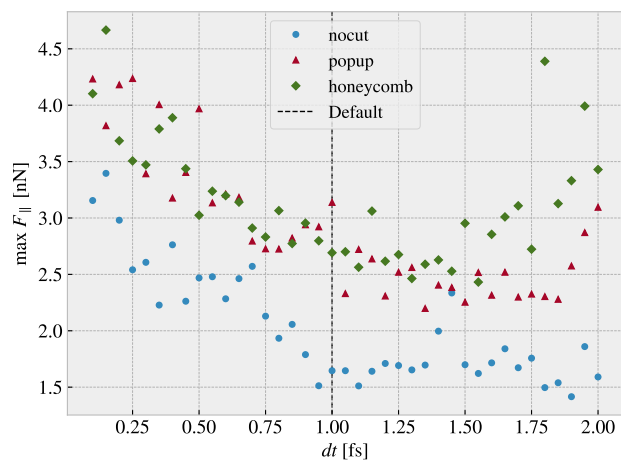
(a) mean friction



(b) max friction

Figure 13: Spring constant

(a) mean friction



(b) max friction

Figure 14: Timestep

0.6.6 Normal force and stretch dependencies

0.6.6.1 Multi stretch

text

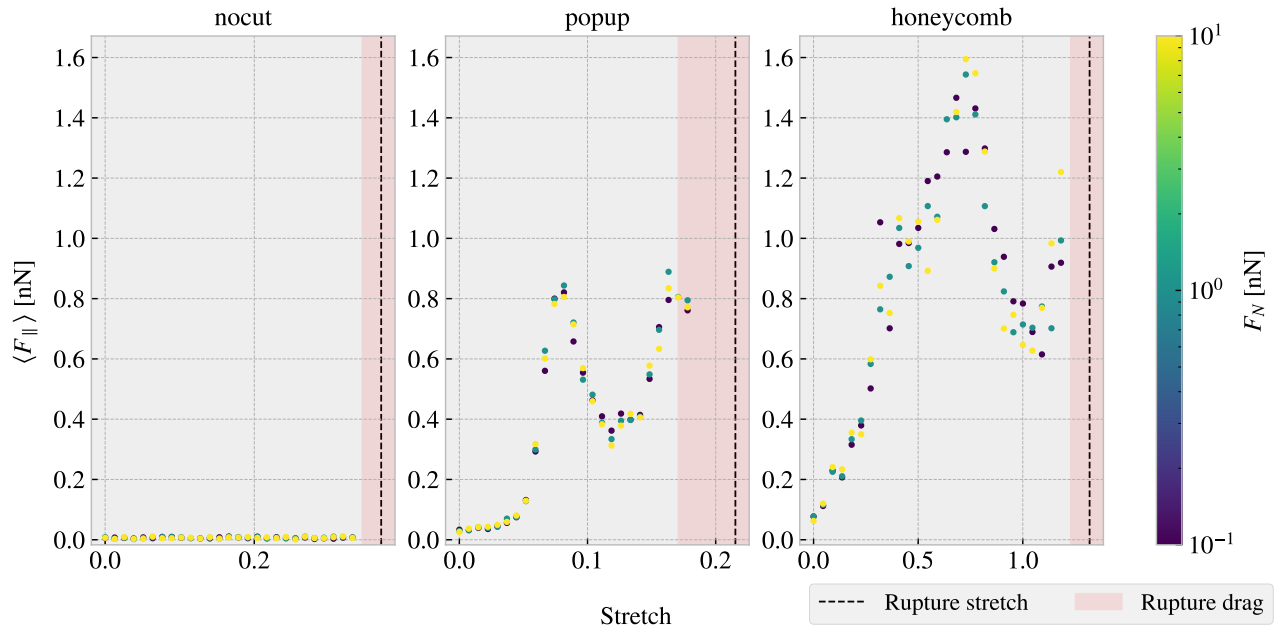


Figure 15: ...

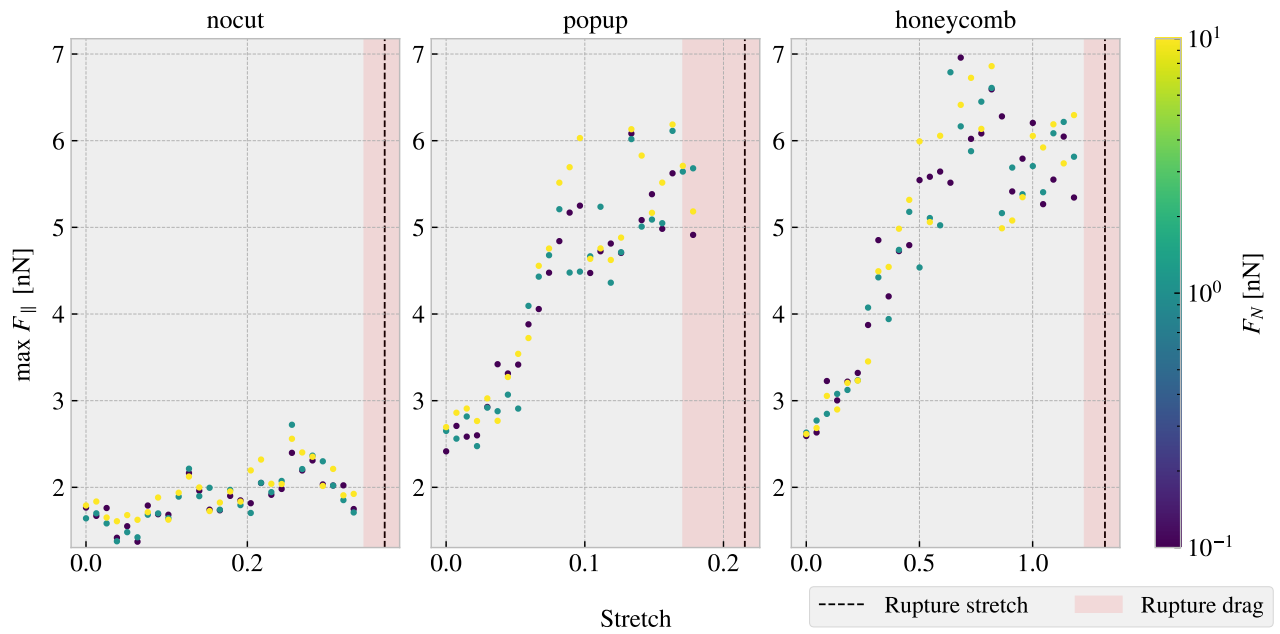


Figure 16: ...

0.6.6.2 Multi normal force

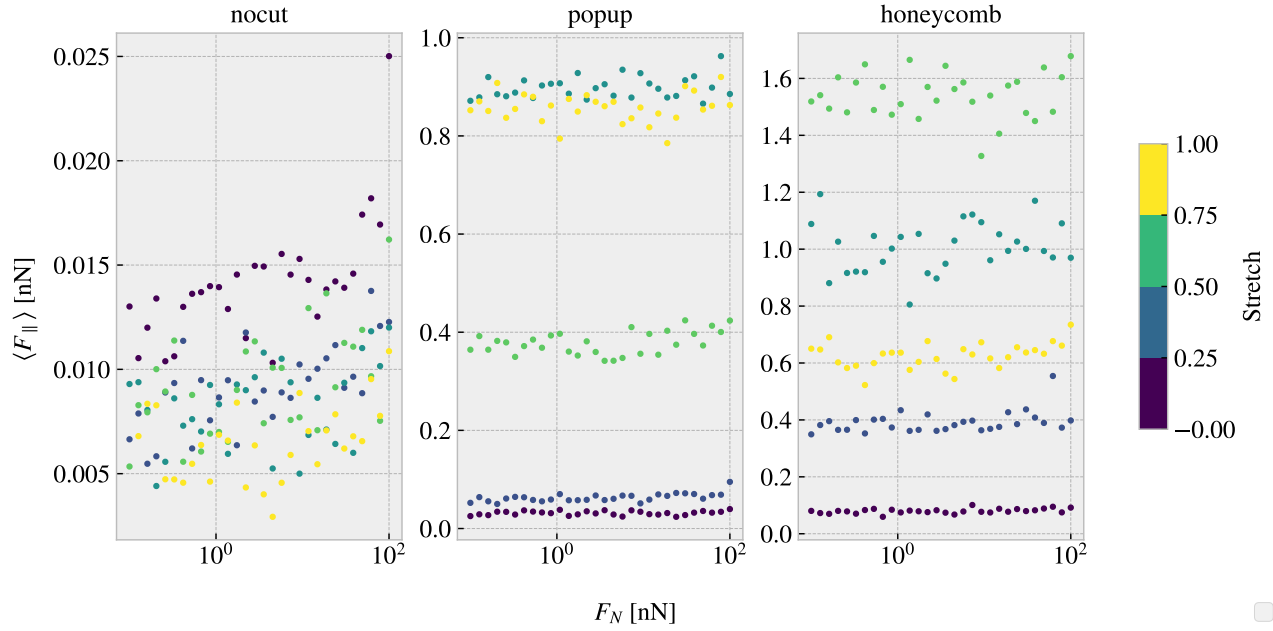


Figure 17: ...

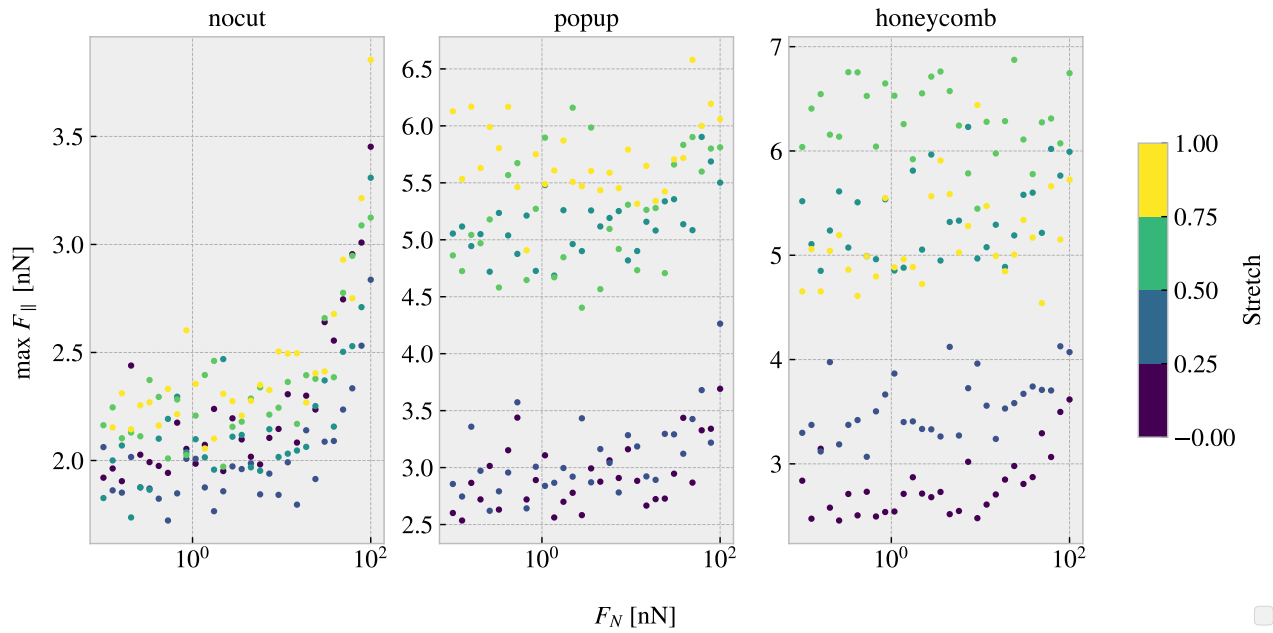


Figure 18: Colorbar is only fitted for the right plot (honeycomb)... this should be fixed. Should I have run a linear distribution of F_N so I could plot it linear here also...?

Table 3: 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 4: Max friction coeff

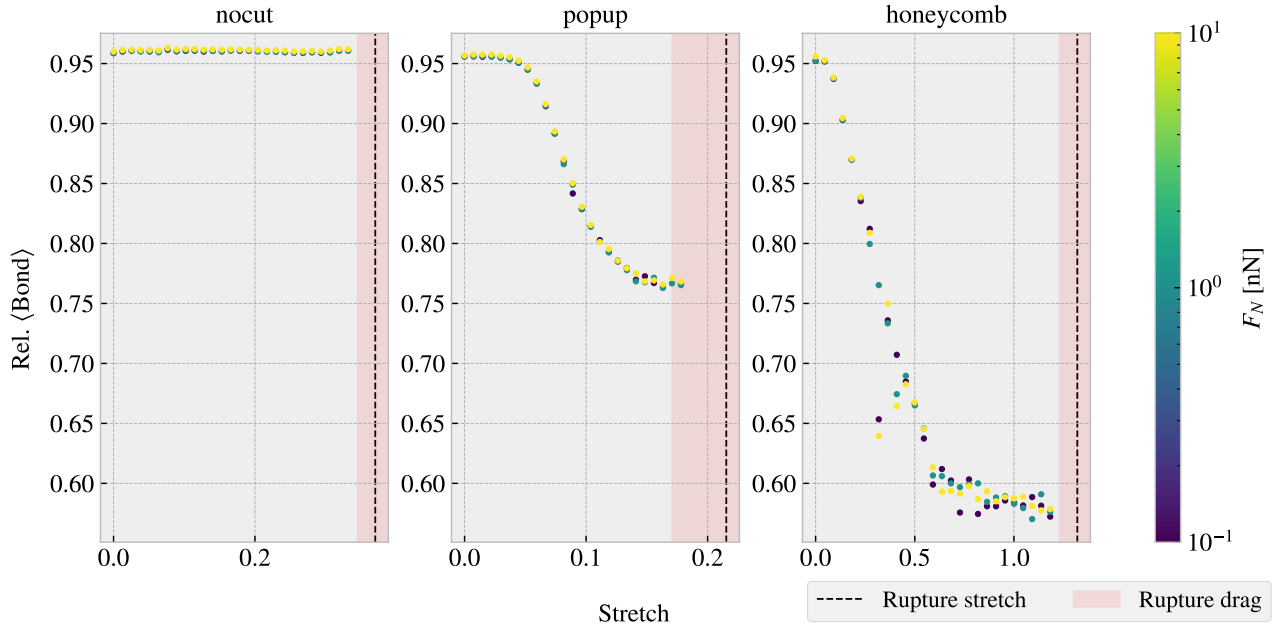
nocut	$0.0139 \pm 9 \times 10^{-4}$	$0.0083 \pm 7 \times 10^{-4}$	$0.010 \pm 1 \times 10^{-3}$	$0.0105 \pm 9 \times 10^{-4}$	
popup	$0.007 \pm 2 \times 10^{-3}$	$0.010 \pm 2 \times 10^{-3}$	$0.007 \pm 2 \times 10^{-3}$	$0.009 \pm 3 \times 10^{-3}$	$0.006 \pm 2 \times 10^{-3}$
honeycomb	$0.010 \pm 1 \times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

The friction probably does not increase with normal force at an expected rate due to the fact 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 so much. By this theory the friction force vs. normal force on the pull graph look a bit more like expected.

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.

0.6.6.3 Contact area

Show plots of contact area vs stretch and discuss the fact that friction actually increases while contact area drops. Is the conclusion that there might be another more dominant cause of the increasing friction.

**Figure 19**

0.6.7 Computational cost

Talk about the computational 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.

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 or something similar.

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 [20](#).

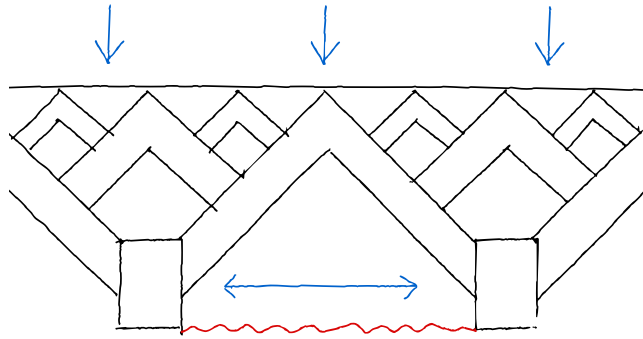


Figure 20: Working sketch for nanomachine

Appendices

Appendix A

Bibliography

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