

Title

Subtitle

by

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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 Some headline for the introtext

Friction is a fundamental physical concept that takes part in almost all thinkable interactions with matter. Even though the everyday person might not be quite familiar with the content of the term “friction” we would undoubtedly notice its disappearing. Without friction it would not be possible to cross a flat surface by foot, lean against the wall without sliding to the floor or even using nails and screws to secure stuff. On the other hand we are not surprised when a moving object comes to a stop when not supplied with yet another push and we know intuitively that sliding down a snow covered hill is much more exiting 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 we seem to take it for granted. We also do not question the fact that solid materials repel other solid materials or similar. However, recognizing the fundamentality and impact of friction we know surprisingly little about the mechanisms behind it (source and or quote here). As a consequence we also have limited knowledge of how to affect friction or whether it is even possible to do so. In an investigation of the potential influence improvement in friction reduction it was reported

“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.” [1].

## 0.2 Introduction to friction and motivation

friction a part of the (wider) field tribology.

- Where is friction important (motivation)
- The economical interest in tribology (quote)
- The missing knowledge about friction.
- What possibilities do we have if we could control friction (friction coefficient).

## 0.3 Introduction to MD simulations and machine learning approaches

The good thing about the process of inverse design is that the uncertainty and missing information from the network (black box) is not important if we are able to locate a working design. Thus we can test the suggested design and remove the doubt of whether this is a good design or not. Thus we do not have to trust the network prediction at all. However, if the predictions are not accurate enough we will most likely never get any useful designs from the ML process, but at least we will be informed whether the designs are good or bad in the end with respect to the simulations. However the question is rather if we can trust the simulation results. In the end we should test the designs in real life to be completely sure and thus the certainty of the quality of any proposed designs is determined by the simulation quality.

## **0.4 Defining the goal of the thesis and restrictions**

Make bullet point objectives for the thesis and state which is completed, which is perhaps not conclusive and which I did not answer at all / do at all. Perhaps also make a list of problems/questions to answer (also state which one I actually answer here).

## **0.5 Contributions**

## **0.6 Thesis structure**



Introduction. A citation to avoid error for now: [2].

- Nanotribology
- Quantitative Structure-Property Relationship
- Forward simulation using ML
- Inverse designs

Practically, systems achieving low values of dry sliding friction are of great technological interest to significantly reduce dissipation and wear in mechanical devices functioning at various scales. (Current trends in the physics of nanoscale friction)

These experiments have demonstrated that the relationship between friction and surface roughness is not always simple or obvious. (Introduction to Tribology, p. 527).

“In other words, it’s not just the material itself” that determines how it slides, but also its boundary condition — including whether it is loose and wrinkled or flat and stretched tight, he says. (<https://news.mit.edu/2016/sliding-flexible-graphene-surfaces-1123>).j– Talking about quality of contact for friciton.



# Chapter 1

## Background Theory and Method

Small introtext to motivate this chapter. What am I going to go over here.

### 1.1 Tribology - friction

#### 1.1.1 Friction on a macroscopic scale - macroscale theories

##### 1.1.1.1 Amontons' law.

The work of Leonardo da Vinci (1452–1519), Guillaume Amontons (1663-705) and Charles de Coulomb (1736-1806) all contributed to what is commonly known as Amontons' law describing the frictional force accuring when starting and keeping a solid block sliding against a solid surface. This emperical law states that the frictional force tangential to the sliding direction is entirely independent of contact area and sliding velocity (at ordinary sliding velocities). Instead it relies only on the normal force  $F_N$  acting from the surface on the block and the material specific friction coefficient  $\mu$  as

$$F_f = \mu F_N.$$

Further it distinguish between *static* and *kinetic* friction as the cases of stationary and sliding contact resepctively. Each type of friction comes with its own friction coefficient,  $\mu_s$  for static and  $\mu_k$  for kinetic friction, usually with values lower than one and  $\mu_s \geq \mu_k$  in all cases. [3][p. 6].

This simple law is a natural starting point for the

Although this model is a common base for understanding friction on a macroscopic level is has its limitations. It turns out that static friction is not constant, but depends on the so-called contact history with increasing friction as the logarithm of time of stationary contact [4]. For the kinetic friction the independency of sliding velocity dissapears at low velocities as thermal effects becomes important and for high velocities due to inertial effetes. [3][pp. 5-6].

It fails to explain the mechanisms behind fritction.

In order to understand what is causing friction between moving objects and how this might result in a linear relationship between friction and normal force we must take the study to a smaller scale... Having an emperical law that seems to predict the friction in many cases leads to the next natural desire for deriving these from fundamental atomic or molecular principles.

#### 1.1.2 Friction on a microscopic scale - Nanotribology

It is generally accepted that friction is caused by two mechanism: mechanical friction and chemical friction. The mechanical friction is the plowing of the surface by hard particles or asperities. The chemical mechanism is adhesion between contacting surfaces. [5].

Sources in general: [6], [5]

### 1.1.2.1 Surface roughness - Asperity theories

Going beyond a macroscopic perspective we realise that most surfaces is in fact rough. The contact between two surfaces consist of numerous smaller contact point, so-called asperities, each with a contact area of  $A_{\text{asp}}$ . The true contact area  $\sum A_{\text{asp}}$  is found to be much smaller than the apperent macroscopic area  $A_{\text{macro}}$ . The friction force is shown to be proportional (extra source on this) to this true contact area as

$$F_f = \tau \sum A_{\text{asp}},$$

where  $\tau$  is an effective shear strength of the contacting bodies. This is still compatible with Amontons' law as long as we differentiate between the macroscopic macroscopic and true area and by having the true contact area dependt linearly on applied normal force.

Thus many studies have focused individual asperities to reveal the relationship between the contact area and normal force (13-15 from [6]). By assuming perfectly smooth asperities with radii of curvature from nanometers to micrometres in size continuum mechanics can be used to predict the deformation of asperities as normal force is applied. A model for non-adhesive contact between homogenous, isotropic, linear elastic spheres was first developed by Hertz (17 [6]), which predicted  $A_{\text{asp}} \propto F_N^{2/3}$ . Later adhesion effects were included in a number of subsequent models, including Maugis-Dugdale theory (18 from [6]), which also predicts a sublinear relationship between  $A_{\text{asp}}$  and  $f_N$  leading to a similar sublinear relationship for  $F_f$  and  $F_N$ .

[6].

### 1.1.2.2 Atomic level friction

On the smallest possible scale, atomic scale, the surfaces does not have structural asperities. Instead atomic level friction is being model as a consequence of the rough potential of the atomic landscape.

### 1.1.2.3 Frenkel-Kontorova-Tomlinson (FKT)

Describes atomic scale friction (not fully accurately though) and gives insight in stick slip motion.

### 1.1.2.4 Commensurate and incommensurate

#### 1.1.2.5 Stick slip

At nanoscales things get a bit more unclear. SFM (explain) experiments have reported (copy sources 5, 6, 21 from [6]) where  $F_f \propto F_N$  or even with these quantities being nearly independent of each other.

In several works by J. Fineberg's group [2-4] the transition from sticking to sliding is characterized by slip fronts propagating along the interface. [7][p. 2].

### 1.1.2.6 Commensurate and incommensurate

As expected, high levels of friction were present in the commensurate positions and extremely low friction was found when the surfaces were incommensurate. (<https://physicsworld.com/a/friction-at-the-nano-scale/>)

### 1.1.2.7 Superlubricity?

Superlubricity, now a pervasive concept of modern tribology, dates back to the mathematical framework of the Frenkel Kontorova model for incommensurate interfaces [40]. When two contacting crystalline workpieces are out of registry, by lattice mismatch or angular misalignment, the minimal force required to achieve sliding, i.e. the static friction, tends to zero in the thermodynamic limit – that is, it can at most grow as a power less than one of the area – provided the two substrates are stiff enough. (Current trends in the physics of nanoscale friction)

Superlubricity is experimentally rare. Until recently, it has been demonstrated or implied in a relatively small number of cases [29, 42–46]. There are now more evidences of superlubric behavior in cluster nanomanipulation [32, 33, 47], sliding colloidal layers [48–50], and inertially driven rare-gas adsorbates [51, 52]. (Current trends in the physics of nanoscale friction)

A breakdown of structural lubricity may occur at the heterogeneous interface of graphene and h-BN. Because of lattice mismatch (1.8%), this interface is intrinsically incommensurate, and superlubricity should persist regardless of the flake-substrate orientation, and become more and more evident as the flake size increases [57]. However, vertical corrugations and planar strains may occur at the interface even in the presence of weak van der Waals interactions and, since the lattice mismatch is small, the system can develop locally commensurate and incommensurate domains as a function of the misfit angle [58, 59]. Nonetheless, spontaneous rotation of large graphene flakes on h-BN is observed after thermal annealing at elevated temperatures, indicative of very low friction due to incommensurate sliding [60, 61]. (Current trends in the physics of nanoscale friction)

Indeed, we know from theory and simulation [74–76] that even in clean wearless friction experiments with perfect atomic structures, superlubricity at large scales may, for example, surrender due to the soft elastic strain deformations of contacting systems. (Current trends in the physics of nanoscale friction)

### 1.1.3 Temperature dependence

Thus, it is commonly expected that the friction of a dry nanocontact should classically decrease with increasing temperature provided no other surface or material parameters are altered by the temperature changes [77, 80–83]. (Current trends in the physics of nanoscale friction)

### 1.1.4 Summary of expected frictional properties

1. Friction should decrease by increasing temperature.
  2. We expect stick slip motion
  3. What about dependence on normal force?
  4. Dependence on contact area?
  5. Dependence on speed?
- Different friction models on macro-and microscopic scale

### 1.1.5 Graphene

Because of this frictional reduction, many studies indicate graphene as the thinnest solid-state lubricant and anti-wear coating [104–106]. (Current trends in the physics of nanoscale friction)

Accurate FFM measurements on few-layer graphene systems show that friction decreases by increasing graphene thickness from a single layer up to 4-5 layers, and then it approaches graphite values [97, 99, 101, 107, 108]. (Current trends in the physics of nanoscale friction)

- General properties and crystal structure

### 1.1.6 Molecular Dynamics

#### 1.1.6.1 Potentials

The choices of potentials used in the MD simulation is mainly based on the on [2] which have a somewhat similar MD friction simulation, the difference being that they impose a Si-tip on the graphene sheet supported by a Si-substrate where we impose drag the whole sheet upon the substrate. Nonetheless this serves as a good anchor for the methodology of the setup. The covalent bonds of C-C in graphene and Si-Si in the substrate is described by the Tersoff and Stillinger–Weber potentials, respectively. A typical 12-6 Lennard–Jones potential is used to describe the van der Waals adhesive interaction between graphene and the substrate.

**General formulation of potentials...?** On a general note we can generalize the n-body potential as the expansion in orders of participating atoms as

$$E = \sum_i V_1(\mathbf{r}_i) + \sum_{\substack{i,j \\ i < j}} V_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_{\substack{i,j,k \\ i < j < k}} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$

where  $\mathbf{r}_n$  is the position of the  $n$ th particle and  $V_m$  is called an  $m$ -body potential [8]. The first one-body term corresponds to an external potential, followed by the two-body term, the three-body term and so on. The simplest model that includes particle interaction is the pair potential truncating the expansion after the two-body term. A general feature of the pair potentials is that they favor close-packed structures which is unsuited to describe covalent bonds that take more open structures. In particular, pair potentials are completely inapplicable to strongly covalent systems such as semiconductors [8]. In order to accommodate the description of covalent bonds the natural step is thus to include the next step of the expansion, the three-body terms, as we will see for the modeling of the graphene sheet C-C bonds and the Silicon sheet Si-Si bonds. For the interaction between the sheet and the substrate we can employ a Lennard Jones pair potential describing the non-bonded van der Waals interaction.

### 1.1.6.2 Lennard Jones

This section is based on [[9], [10], [11]].

The Lennard-Jones (LJ) model is probably one of the most famous pair potentials used in MD simulations. LJ models the potential energy between two non-bonding atoms based solely on interatomic distance  $r$ . The model accounts for attractive forces arising from dipole-dipole, dipole-induced dipole and London interactions, and repulsive forces that capture the hard core (is this safe to say?) of overlapping wave functions at small distances. Thus it is assumed neutrally charged atoms and was originally proposed for noble gases. The classical 12-6 version of the model (referring to the power law of the repulsive and attractive forces respectively) reads

$$E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \quad r < r_c, \quad (1.1)$$

where  $r$  is the interatomic distance with cut-off  $r_c$ ,  $\epsilon$  is the depth of the potential well and  $\sigma$  the distance where the potential is zero. By solving for the potential minimum ( $dE/dr = 0$ ) we find the equilibrium distance to be  $r_0 = \sigma 2^{1/6}$ . This makes for an even clearer interpretation of  $\sigma$  which effectively sets the equilibrium distance between atoms, i.e. the dividing line for which the net force is repulsive or attractive. While the LJ model in many ways is an oversimplified model that is insufficient in its description of ... (get source and concrete examples) it is commonly used as a model for intermaterial interactions (between moving object and substrate) in friction studies [[2], [12], [5]].

### 1.1.6.3 Stillinger weber

This section is based on [[13], [14]]

The stillinger weber potential takes the form of a three body potential

$$E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk}),$$

where  $r_{ij}$  denotes the distance between atom  $i$  and  $j$  and  $\theta_{ijk}$  the angle between bond  $ij$  and  $jk$ . The summations are over all neighbours  $j$  and  $k$  of atom  $i$  within a cut-off distance  $r = a\sigma$ .

The two-body term  $\phi_2$  builds from the LJ model with the addition of an exponential cutoff term

$$\phi_2(r_{ij}) = A_{ij}\epsilon_{ij} \left[ B_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{p_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{q_{ij}} \right] \exp \left( \frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}} \right). \quad (1.2)$$

The model parameters  $A$ ,  $\epsilon$ ,  $B$ ,  $\sigma$ ,  $p$ ,  $q$  and  $a$  comes with  $i, j$  indices to indicate that these parameters should be specified for each unique pair of atom types. However, in our case we will only provide a single value for each model parameter as we are exclusively dealing with Si-Si bonds. We see that the first term in eq. (1.2) is reminiscent of the LJ model in eq. (1.1) while the last term effectively drives the potential to zero at  $r = a\sigma$ ,

which is thus the chosen cut-off distance for the potential evaluation. With the model parameters for the Si-Si modelling (see table 1.1) the cut-off becomes  $\sim 3.8$  Å.

The three body term includes an angle dependency as

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk} \epsilon_{ijk} \left[ \cos \theta_{ijk} - \cos \theta_{0,ijk} \right]^2 \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right) \exp\left(\frac{\gamma_{ik}\sigma_{ik}}{r_{ik} - a_{ik}\sigma_{ik}}\right), \quad (1.3)$$

where  $\theta_{0,ijk}$  is the equilibrium angle. The first term of eq. (1.3) includes an angle dependency analog to a harmonic oscillator based on a cosine angle distance from the equilibrium angle. The final two terms act again as a cut-off function by driving the potential to zero at  $r_{ij} = a_{ij}\sigma_{ij}$  and  $r_{ik} = a_{ik}\sigma_{ik}$  respectively.

The parameters used for the Si-Si bond modeling is displayed in table 1.1 along with an interpretation of each model parameter.

**Table 1.1:** Parameters for the stilliner weber potential used for intermolecular interactions in the silicon substrate.

Parameter	Value	Description
$\epsilon$	2.1683	Individual depth of the potential well for each atom type pair/tiplets.
$\sigma$	2.0951	Distance for which the individual pair interactions has zero potential (analog to the LJ model).
$a$	1.80	The individual cut-off distance for each atom type pair.
$\lambda$	21.0	The overall depth of the three-body potential well.
$\gamma$	1.20	The shape of the three-body cut-off terms.
$\cos(\theta_0)$	-1/3	Cosine of equilibrium angle.
$A$	7.049556277	The overall depth of the two-body potential well.
$B$	0.6022245584	Scales the repulsion part of the two-body term.
$p$	4.0	The power dependency for the repulsion part of the two-body term.
$q$	0.0	The power dependency for the attraction part of the two-body term.
tol	0.0	LAMMPS: Option to define a different cut-off than the theoretical of $r = a\sigma$ . $tol = 0$ refers to the theoretical being used.

#### 1.1.6.4 Tersoff

This section is based on [[15], [8]].

The tersoff potential abandon the idea of a general  $n$ -body form and attempts instead to build the model on a more physics informed approach; The more neighbours an atom has the weaker the bonds will be. Thus it introduces the bond order (bond strength), that is environment specific and decrease with increasing bond coordination (number of neighbours for a given atom). The potential energy is taken to have the form

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij},$$

$$V_{ij} = f_C(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})],$$

where the total potential energy is decomposed into a bond energy  $V_{ij}$ . The indices  $i$  and  $j$  run over the atoms of the system with  $r_{ij}$  denoting the distance between atom  $i$  and  $j$ . Notice that the sum includes all combinations of  $i, j$  where  $i \neq j$  meaning that the same bond is double counted which is the reason for the additional factor 1/2. The reasoning behind comes from the asymmetry of the bond order  $b_{ij} \neq b_{ji}$  leading to a  $V_{ij} \neq V_{ji}$ . The bond energy is composed of a repulsive term  $f_R$ , arising from overlapping wave functions, and an attractive term  $f_A$  associated with bonding.  $f_C$  is simply a smooth cut-off function to increase computational efficiency.  $b_{ij}$  represent the bond order, i.e. the strength of the bonds, which depends inversely on the number of bonds, the bond angles ( $\theta_{ijk}$ ) and optionally the relative bonds lengths ( $r_{ij}, r_{jk}$ ). Notice that an additional

cut-off term  $a_{ij}$  was originally multiplied to  $f_R$  as a way of including terms that limit the range of the interactions to the first neighbour shell. These kind of limitations is already included in  $b_{ij}$  for the attractive term  $f_A$  but is often omitted for the repulsive term  $f_R$ , and we do so to by setting  $a_{ij} = 1$ . The cut-off function  $f_C$  goes from 1 to 0 over a small interval range  $R \pm D$  as

$$f_C(r) = \begin{cases} 1 & r < R - D \\ \frac{1}{2} - \frac{1}{2} \sin\left(\frac{\pi}{2} \frac{r-R}{D}\right) & R - D < r < R + D, \\ 0 & r > R + D \end{cases}$$

which is continuous and differentiable for all  $r$ .  $R$  is usually chosen to include only the first neighbour shell. The repulsive and attractive terms  $f_R$  and  $f_A$  is modelled as an exponetial function, similar to a morse potential,

$$\begin{aligned} f_R(r) &= A \exp(-\lambda_1 r), \\ f_A(r) &= -B \exp(-\lambda_2 r). \end{aligned}$$

The novel feature of the model lies in modeling of the bond order  $b_{ij}$  which includes three-body interactions by summing over a third atom  $k \neq i, j$  within the cut-off  $r_{ik} < R + D$  as shown in the following.

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-\frac{1}{2n}} \quad (1.4)$$

$$\zeta_{ij} = \sum_{k \neq i, j} f_C(r_{ik}) g(\theta_{ijk}(r_{ij}, r_{ik})) \exp(\lambda_3^m (r_{ij} - r_{ik})^m) \quad (1.5)$$

$$g(\theta) = \gamma_{ijk} \left( 1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos \theta - \cos \theta_0)^2]} \right). \quad (1.6)$$

In eq. (1.6)  $\zeta_{i,j}$  is an effective coordination and  $g(\theta)$  captures angle dependency as it is minimized at the equilibrium angle  $\theta = \theta_0$ .

The parameters used to model the graphene C-C bonds is summarized in table 1.2

**Table 1.2:** Parameters for the tersoff potential used for intermolecular interations in the graphene sheet

Parameter	Value	Description
$m$	3.0	Default (not used since $\lambda_3 = 0$ )
$\gamma$	1.0	...
$\lambda_3$	$0.0 \text{ \AA}^{-1}$	...
$c$	$3.8049 \times 10^4$	Strength of the angular effect
$d$	4.3484	Determines the “sharpness” of the angular dependency
$\cos(\theta_0)$	-0.57058	Cosine of the equilibrium angle
$n$	0.72751	Power law exponent for the bond order dependency
$\beta$	$1.5724 \times 10^{-7}$	...
$\lambda_2$	$2.2119 \text{ \AA}^{-1}$	Decay of repulsion potential term
$B$	346.74 eV	Attractive potential term minimum at core ( $r_{ij} = 0$ ).
$R$	$1.95 \text{ \AA}$	Center distance for cut-off
$D$	$0.15 \text{ \AA}$	Thickness of cut-off layers
$\lambda_1$	$3.4879 \text{ \AA}^{-1}$	Decay of repulsion potential term
$A$	1393.6 eV	Repulsion potential term at core ( $r_{ij} = 0$ )

### 1.1.6.5 LAMMPS

### 1.1.6.6 Integration

Solving newtons equations of motion



$$\ddot{x}(t) = \frac{F(x)}{m} \rightarrow \dot{x} = v(t), \quad \dot{v}(t) = \frac{F(x(t))}{m}$$

Integration of newtons equations of motion (just like, Euler, Euler cromer and so on) and specify the verlet algorithm which is used in Lammmps.

The forces (form the potential) is conservative so the energy should be conserved before applying the thermostat.

However small erros applied by the discrete integratiton algorithm we end up having an energy error. This is sensitive to time step.

**Velocity Verlet** The velocity verlet algorithm can be derived by taken a number of taylor expansion. We begin by expanding the next step position vector  $\mathbf{x}(t + \Delta t)$  around time  $t$

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \dot{\mathbf{x}}\Delta t + \frac{\ddot{\mathbf{x}}}{2}(\Delta t)^2 + \mathcal{O}((\Delta t)^3) \quad (1.7)$$

Similar we take the expansions of the next step velocity vector  $\mathbf{v}(t + \Delta t)$  at time  $t$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \dot{\mathbf{v}}(t)\Delta t + \frac{\ddot{\mathbf{v}}(t)}{2}(\Delta t)^2 + \mathcal{O}((\Delta t)^3) \quad (1.8)$$

By also taking the taylor expansion of  $\dot{\mathbf{v}}(t + \Delta t)$  we can eliminate the  $v\ddot{e}c v$  term in eq. (1.8) as done in the following.

$$\begin{aligned} \dot{\mathbf{v}}(t + \Delta t) &= \dot{\mathbf{v}}(t) + \ddot{\mathbf{v}}(t)\Delta t + \mathcal{O}((\Delta t)^2) \\ \frac{\ddot{\mathbf{v}}(t)}{2}(\Delta t)^2 &= \frac{\Delta t}{2} \left( \dot{\mathbf{v}}(t + \Delta t) - \dot{\mathbf{v}}(t) \right) + \mathcal{O}((\Delta t)^3) \\ &\Downarrow \\ \mathbf{v}(t + \Delta t) &= \mathbf{v}(t) + \dot{\mathbf{v}}(t)\Delta t + \frac{\Delta t}{2} \left( \dot{\mathbf{v}}(t + \Delta t) - \dot{\mathbf{v}}(t) \right) + \mathcal{O}((\Delta t)^3) \\ &= \mathbf{v}(t) + \frac{\Delta t}{2} \left( \dot{\mathbf{v}}(t) + \dot{\mathbf{v}}(t + \Delta t) \right) + \mathcal{O}((\Delta t)^3) \end{aligned} \quad (1.9)$$

By combining eq. (1.7) and eq. (1.9) while cleaning up the notation using  $\mathbf{v} = \dot{\mathbf{x}}$  and  $\mathbf{a} = \dot{\mathbf{v}}$  we get the final scheme

$$\begin{aligned} \mathbf{x}(t + \Delta t) &= \mathbf{x}(t) + \mathbf{v}(t)\Delta t + \frac{\mathbf{a}(t)}{2}(\Delta t)^2 + \mathcal{O}((\Delta t)^3), \\ \mathbf{v}(t + \Delta t) &= \mathbf{v}(t) + \frac{\mathbf{a}(t) + \mathbf{a}(t + \Delta t)}{2}\Delta t + \mathcal{O}((\Delta t)^3). \end{aligned}$$

The scheme will give a local error of order  $(\Delta t)^3$  corresponding to a global error of  $(\Delta t)^2$ . Lets descritize the time as  $t_k = k * \Delta t$  with position  $\mathbf{x}_k$  and velocity  $\mathbf{v}_k$ . At time  $t_k$  the acceleration is given  $\mathbf{a}_k = F(\mathbf{x}_k)/m$ . We get the implementation steps as follows

1. Calculate  $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{v}_k\Delta t + \frac{F(\mathbf{x}_k)}{2m}$
2. Evaluate  $F(\mathbf{x}_{k+1})$
3. Calculate  $\mathbf{v}_{k+1} = \mathbf{v}_k + \frac{F(\mathbf{x}_k) + F(\mathbf{x}_{k+1})}{2m}\Delta t$

### 1.1.6.7 Thermostats

This section is based on [16], [17](pp. 115, 120-121) and [18]

In order to simulate the canonical ensemble, that is the ensemble defined by a constant amount of particles  $N$ , constant temperature  $T$  and constant volume  $V$ , hence often denoted  $NVT$ , we apply a so-called thermostat. There exist a variety of such including Nosé-Hoover, Gaussian, Berendsen, Langevin thermostat and many other (give example of how they modify) We will use the ladder.

The connical ensemble is an ensemble of systems by the assumption that the system of interests is connected to an infitely large heat bath of temperature  $T$ . The Langevin thermostat assumes that the particles collides with much smaller lighter particles representing the heat bath as a sea of small particles. The collisions is described by a friction force  $f_f = -\gamma \mathbf{p}$ , where  $\gamma$  is positiv friction coefficient and  $\mathbf{p}$  the momentum vector, and a random force  $f_r = \mathbf{R}_i(t)$ . By denoting the conservative force arising from the usual inter-particle interactions  $\mathbf{f}_i$  on particle  $i$  we get the Langevin equations of motion describing the total force  $\mathbf{F}_i$  on particle  $i$  as

$$\begin{aligned}\mathbf{F}_i &= \mathbf{f}_i + \mathbf{f}_{f,i} + \mathbf{f}_{r,i} \\ m_i \ddot{\mathbf{r}}_i &= \mathbf{f}_i - \gamma_i \mathbf{p}_i + \mathbf{R}_i(t)\end{aligned}\tag{1.10}$$

where  $m_i$  is the mass of particle  $i$   $\mathbf{r}_i$  the position vector. The random force  $\mathbf{R}_i(t)$  is described as gaussian white noise and have the following properties.

1. It is uncorrelated with the velocities  $\dot{\mathbf{r}}(t)$  and deterministic forces  $\mathbf{f}_i(t')$  at previous times  $t' < t$ .
2. The time average is zero:  $\langle \mathbf{R}(t) \rangle = \mathbf{0}$ .
3. The mean-square components evaluate to  $2m_i\gamma_i k_B T$ .
4. The force component of particle  $i$   $R_{i,\mu}$  along cartesian axis  $\mu$  is uncorrelated with any component of particle  $j$   $R_{j,\nu}$  along cartesian axis  $\nu$ , unless  $i = j$ ,  $\mu = \nu$  and  $t = t'$ .

The ladder two conditions can be formulated as

$$\langle R_{i,\mu}(t) R_{j,\nu}(t') \rangle = 2m_i\gamma_i k_B T \delta_{ij} \delta_{\mu\nu} \delta(t' - t),$$

where  $\delta_{..}$  is the Kronecker Delta function and  $\delta(\cdot)$  is the Dirac Delta function. It can be shown that a trajectory generated by integrating the Langevin equations of motion (eq. (1.10)) maps a cononical distribution of microstates at temperature  $T$ . [17](p.121).

In practice the implementation of the thermostat is implemented discretely by updating the force on each particle by the addition of the described forces  $f_f$  and  $f_r$  for each particle. In LAMMPS this is controlled by the user defined damping factor “damp” =  $\gamma^{-1}$  in units of time whih control how fast we are going to reach the temperature equilibrium. Thus the documentation ([18]) defines the added forces as

$$f_f = -\frac{m}{\text{damp}}, \quad f_r \propto \sqrt{\frac{mk_B T}{dt \text{ damp}}}$$

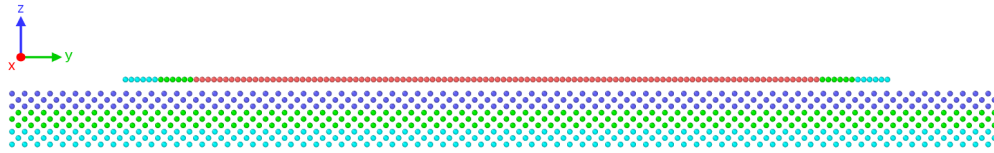
where  $v = \dot{r}$  is the velocity. The definition of  $f_f$  falls straight out of the definition above in eq. (1.10) while the proportionality of  $f_r$  comes from

$$\sqrt{\langle R(t)^2 \rangle} = \sqrt{2m\gamma k_B T} \propto \sqrt{\frac{mk_B T}{\text{damp}}}$$

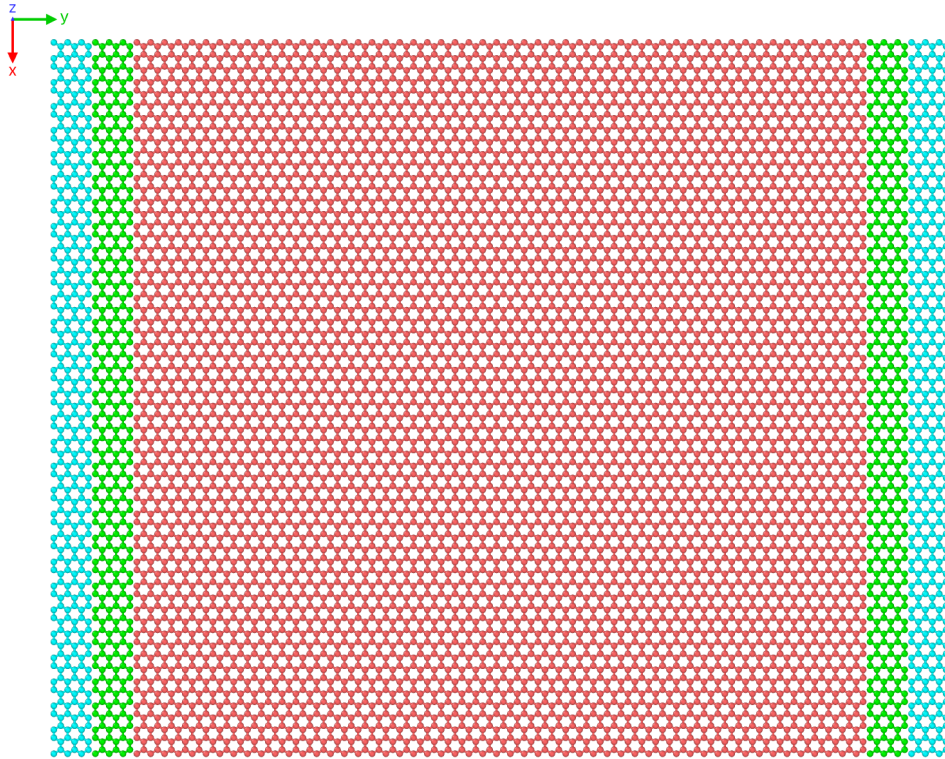
Thus we have  $f_r \propto \sqrt{\langle R(t)^2 \rangle / dt}$  which I do not quite understand. It is mentioned in <https://pubs.acs.org/doi/full/10.1021/ct8002173> when talkikng about residual forces, as it is natural when taking a step length of  $dt...$  Probably simply, but check this later.

### 1.1.7 Defining the system

Include figure of system to point out thermo layers and freeze layers.



(a) Side view



(b) Top view

**Figure 1.1:** System. 27456 atoms in total: 7272 with thermostat (orange), 7272 is locked (light blue) and the remaining 12912 just with NVE. (Get better colors)

**Table 1.3:** System atom count and region division.

Region	Total	Sub region	Sub total	NVE	NVT	Locked
Sheet	7800	Inner sheet	6360	6360	0	0
		Pull blocks	1440	0	720	720
Substrate	19656	Upper	6552	6552	0	0
		Middle	6552	0	6552	0
		Bottom	6552	0	0	6552
All	27456			12912	7272	7272

### 1.1.8 Creating sheets

We are going to create a 2D sheet graphene sheet.

#### 1.1.8.1 Graphene

Graphene is a single layer of carbon atom, graphite is the bulk, arranged in a hexagonal lattice structure. We can describe the 2D crystal structure in terms of its primitive lattice vector and a basis. That is we populate each lattice site by the given basis and translate it to fill the whole plane by any linear combination of the lattice vectors

$$\mathbf{T}_{mn} = m\mathbf{a}_1 + n\mathbf{a}_2, \quad m, n \in \mathbb{N}.$$

For graphene we have the primitive lattice vectors

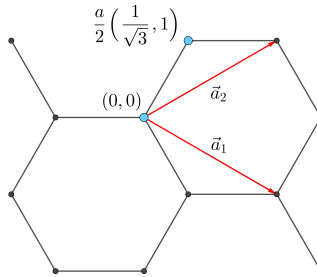
$$\mathbf{a}_1 = a \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right), \quad \mathbf{a}_2 = a \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right), \quad |\mathbf{a}_1| = |\mathbf{a}_2| = 2.46 \text{ \AA}.$$

Notice that we deliberately excluded the third coordinate as we only consider a single graphene layer on not the bulk graphite consisting of multiple layers stacked on top of each other. The basis is

$$\left\{ (0, 0), \frac{a}{2} \left( \frac{1}{\sqrt{3}}, 1 \right) \right\}$$

It turns out that the spacing between atoms is equal for all pairs with an interatomic distance

$$\left| \frac{a}{2} \left( \frac{1}{\sqrt{3}}, 1 \right) \right| \approx 1.42 \text{ \AA}.$$



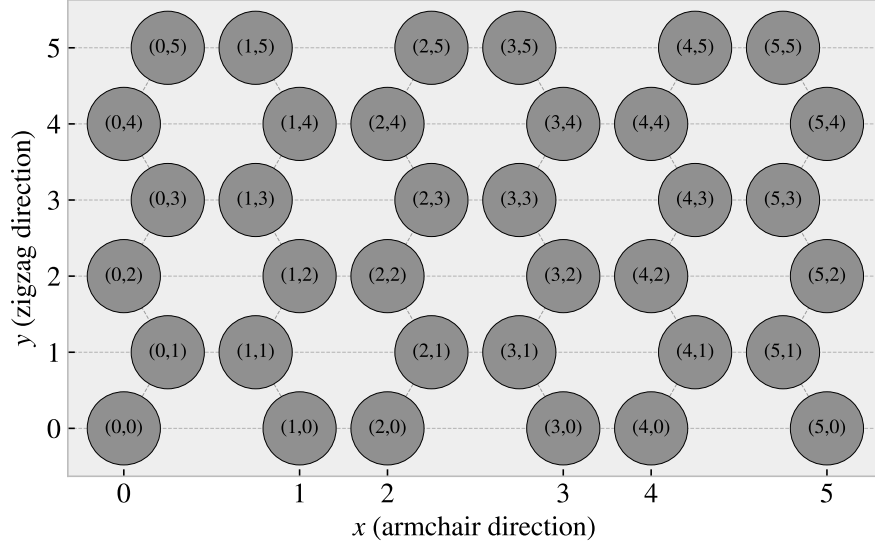
**Figure 1.2:** Graphene crystal structure with basis.

#### 1.1.8.2 Indexing

In order to define the cut patterns applied to the graphene sheet we must define an indexing system. We must ensure that this gives a unique description of the atoms as we eventually want to pass a binary matrix, containing 0 for removed atom and 1 for present atom, that uniquely describes the sheet. We do this by letting the x-coordinate point to zigzag chains and the y-coordinate to the position along that chain. This is illustrated in figure 1.3. Other solutions might naturally involve the lattice vectors, but as these only can be used to translate to similar basis atoms a unfortunate duality is introduced as ones need to include the basis atom of choice into the indexing system. With the current system we notice that locality is somewhat preserved. That is, atom  $(i, j)$  is in the proximity of  $\{(i+1, j), (i-1, j), (i, j+1), (i, j-1)\}$ , but only three of them is categorized as nearest neighbours due to the hexagonal structure of the lattice. While  $(i, j \pm 1)$  is always nearest neighbours the

neighbour in the x-direction flip sides with incrementing y-coordinate. That is the nearest neighbours (NN) is decided as

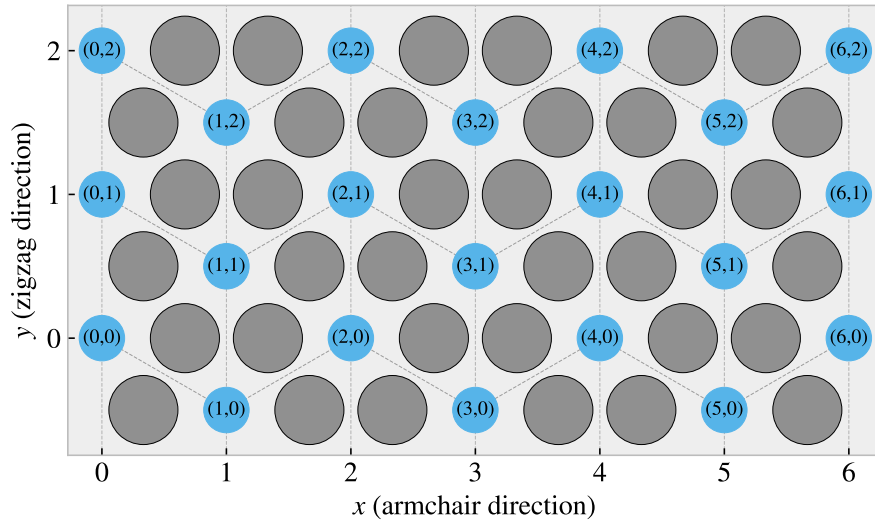
$$\begin{aligned} j \text{ is even} &\rightarrow \text{NN} = \{(i+1, j), (i, j+1), (i, j-1)\}, \\ j \text{ is odd} &\rightarrow \text{NN} = \{(i-1, j), (i, j+1), (i, j-1)\}. \end{aligned}$$



**Figure 1.3:** Graphene atom indexing

### 1.1.8.3 Removing atoms

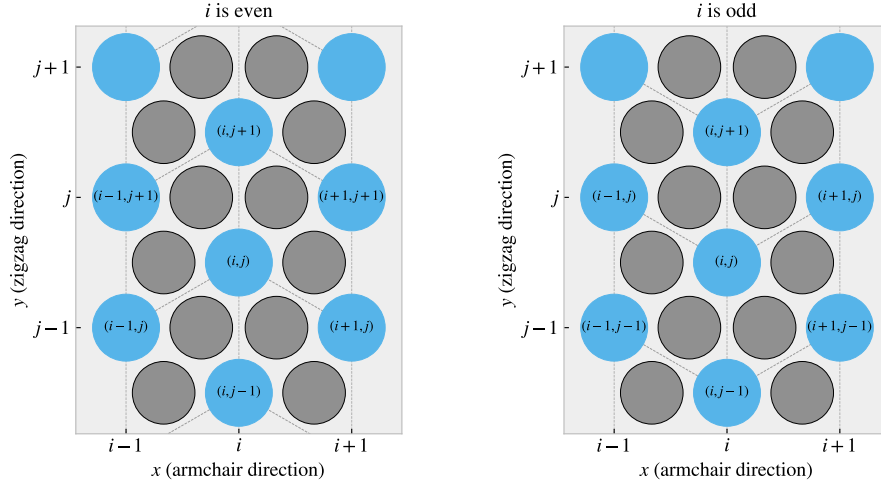
As a mean to ease the formulation of cut patterns we introduce pseudo center element in each gap of the hexagonal honeycombs, see figure 1.4.



**Figure 1.4:** Graphene center indexing

Similar to the case of the indexing for the carbon atoms themselves the nearest neighbour center elements alternate with position, this time along the x-coordinate. Each center element has six nearest neighbours, in clock wise direction we can denote them: “up”, “upper right”, “lower right”, “down”, “lower left”, “upper left”.

The “up” and “down” is always accessed as  $(i, j \pm 1)$ , but for even  $i$  the  $(i + 1, j)$  index corresponds to the “lower right” neighbour while for odd  $i$  this corresponds to the “upper right” neighbour. This shifting applies for all left or right neighbours and the full neighbour list is illustrated in figure 1.5.



**Figure 1.5:** Graphene center elements directions

We define a cut pattern by connecting center elements into connected paths. As we walk element to element we remove atoms according to one of two rules

1. Remove intersection atoms: We remove the pair of atoms placed directly in the path we are walking. That is, when jumping to the “up” center element we remove the two upper atoms located in the local hexagon of atoms. This method is sensitive to the order of the center elements in the path.
2. Remove all surrounding atoms: We simply remove all atoms in the local hexagon surrounding each center element. This method is independent of the ordering of center elements in the path.

We notice that removing atoms using either of these rules will not guarantee an unique cut pattern. Rule 1 is the more sensitive to paths but we realize that, for an even  $i$ , we will remove the same five atoms following either of the following paths.

$$\begin{aligned}
 (i, j) &\rightarrow \underbrace{(i+1, j+1)}_{\text{upper right}} \rightarrow \underbrace{(i, j+1)}_{\text{up}} \rightarrow \underbrace{(i+1, j+2)}_{\text{upperright + up}} \rightarrow \underbrace{(i+1, j+1)}_{\text{upper right}} \\
 (i, j) &\rightarrow \underbrace{(i+1, j+1)}_{\text{upper right}} \rightarrow \underbrace{(i+1, j+2)}_{\text{upperright + up}} \rightarrow \underbrace{(i, j+1)}_{\text{up}}
 \end{aligned}$$

For rule 2 it is even more obvious that different paths can result in the same atoms being removed. This is the reason that we needed to define an indexing system for the atom position itself even though that all cuts generated manually will use the center element path as reference.

Illustrate some delete path?

#### 1.1.8.4 Pull blocks

### 1.1.9 Kirigami inspired cut out patterns

#### 1.1.9.1 Pop-up pattern

#### 1.1.9.2 Honeycomb

#### 1.1.9.3 Random walk

- MD simulation (classical or ab initio)
- Basics of classical MD simulations: Integration and stuff
- Ab initio simulation (quantum mechanics, solving schrödinger)

### 1.1.10 Real life experimental procedures

From Introduction to Tribology, Second Edition, p. 526:

The surface force apparatus (SFA), the scanning tunneling microscopes (STM), and atomic force and friction force microscopes (AFM and FFM) are widely used in nanotribological and nanomechanics studies.

- Real life procedures to mimic in computation, for instance Atomic Force Microscopy (AFM) for friction measurements.
- Available technology for test of my findings if successful (possibilities for making the nano machine)

### 1.1.11 Machine Learning (ML)

- Feed forward fully connected
- CNN
- GAN (encoder + decoder)
- Genetic algorithm
- Using machine learning for inverse designs partly eliminate the black box problem. When a design is produced we can test it, and if it works we not rely on machine learning connections to verify it's relevance.
- However, using explainations techniques such as maybe t-SNE, Deep dream, LRP, Shapley values and linearizations, we can try to understand why the AI chose as it did. This can lead to an increased understanding of each design feature. Again this is not dependent on the complex network of the network as this can be tested and verified independently of the network.

### 1.1.12 Feed forward network / Neural networks

### 1.1.13 CNN for image recognition

### 1.1.14 GAN (encoder + deoder)

### 1.1.15 Inverse desing using machine learning

### 1.1.16 Prediction explanation

#### 1.1.16.1 Shapley

#### 1.1.16.2 Lineariations

#### 1.1.16.3 LRP

#### 1.1.16.4 t-SNE





# Method

## 1.2 Free floating bullet points to remember

- Describe two different approaches:
  - Nanomachine setup (sheet as the inner layer of nanomachine influencing the stretch)
  - Graphene skin setup (sheet on the outside probed with tip, stretched and fixed on object)

## 1.3 Setting up the system

- Substrate material (crystalline or amorphous)
- Intra- and intermolecular potentials
- Ensembles: NVE, NVT
- Choice of dt, relax time etc.

## 1.4 Measuring properties

- Out-of-plane buckling
- Contact area
- Friction (static, dynamic)

## 1.5 Making cuts in graphene

- Indexing the sheet
- Manual patterns as a starting point (Pop-up pattern and half octans)
- Cut rules and problems with dangling fringes
- Different variations of manual patterns
- Random walks

## 1.6 Simulation procedures

- Relaxing
- Stretching
- Friction
- Different combinations of stretch and applied normal force

## 1.7 Working title: tweeking simulation settings

- Substrate structure
- Drag speed
- Spring stiffness
- ...

## 1.8 Handling ruptures

Considered the following parameters to define rupture events.

- Stress (in stretch direction) drop
- Max velocity peak (peak in cummax divided by std)
- peak in value MSD (com ave)
- Drop in coordination number
- Number of clusters (should be constant 1). This is the most secure one

Ideally one would store the nearest neighbours for each atom and check that those neighbours stay in proximity during the simulation. This would capture even the smallest rupture, but this is not available at runtime in LAMMPS which made it non ideal. In addition this calculation would also be computationally heavy because of the algorithm needed to make this investigation but also considering the fact that we cannot due early stopping and thus need to run a lot of ruptured sheet to the end of the simulation time.

## 1.9 Sampling data

- Different drag angles

## 1.10 Machine learning

- Input: atom position matrix
- Target properties: friction coefficient (low/high), maybe load curve for nonlinear relations
- Output: Cut pattern, stretch amount (%)
- Architecture and network types
- Loss function and evaluation

Big lines

- Make indexing system/ description of the sheet
- Collect data
  - pop-up pattern
  - RN walk
  - RN straight cuts?
  - RN single atoms removes
  - Rules for patterns
- Train machine learning algorithm to predict properties
  - Static/Dynamic friction coefficient from atom matrix.

Possible subjects

- Indexing the graphene sheet
- Creating a pop-up pattern
- Potentials and materials
- Creating substrate
  - quenching
- Creating data sets
  - random walk?

## Things to remember

- Word: Nanotribology

## Choosing material and potentials

Looking at <https://aip.scitation.org/doi/pdf/10.1063/1.481208>.

The main material of study is the graphene sheet. Graphene is simply a single layer of graphite. For the friction study we need a substrate and a tip which pushes down into the sheet. For the tip and substrate we have considered both diamond and silicon. Here we look at tersoff, REBO and Airebo as possible potentials candidates for intramolecular potentials. For the intermolecular potential we can use a typical 12-6 Lennard-Jones (LJ) potential. Could also choose exp-6 potential which is slightly more complex I think. The repulsive wall is known to be quite hard. Above article is talking about a LJ switch to overcome the hard repulsive wall.

The LJ potential is taking from <https://pubs.rsc.org/en/content/articlehtml/2015/nr/c4nr07445a> referring to <https://journals.aps.org/prb/pdf/10.1103/PhysRevB.81.155408>.

## Work in progress simulation setup

Silicon substrate (crystalline or amorphous) with a single graphene sheet resting on top. A Si tip apex described as a rigid body connected to a moving support (with no atomic interaction) via a harmonic spring to drag the tip apex across the sheet.

Step 1: Load the tip with a normal force such that the tip begin to interact with the sheet. Step 2: Drag the tip in the horizontal direction and measure either static or dynamic friction.

## Find right timestep

From article (Nanoscratching of multi-layer graphene): The equations of particles motion were solved using the Verlet algorithm, and the simulation time step is 1 fs, which is adequate for system relaxation by examining the stability through the root mean square deviations of the atoms.



# Simulations

## Frictional properties of the intact graphene sheet

The friction measurement simulation is governed by the following parameters, which is divided into three sub categories for the purpose of this thesis as shown in table [1.4](#).

**Table 1.4:** Parameters of the numerical procedure for measuring friction.

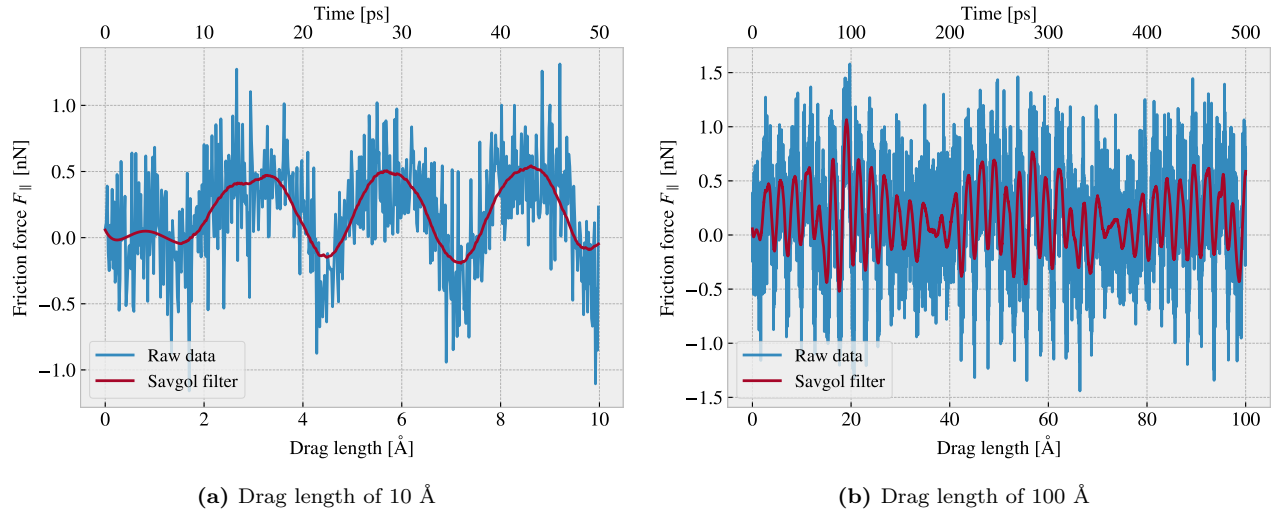
Category	Parameter name: description	Category purpose
Physical	<ul style="list-style-type: none"> <li>- <math>T</math>: Temperature for the Langevin thermostat.</li> <li>- <math>v_{drag}</math>: Drag speed for the sheet translation.</li> </ul>	Parameters that we expect to have an inevitably effect on the system friction properties, for which the choice will be a baseline for our studies.
Measurement	<ul style="list-style-type: none"> <li>- <math>dt</math>: Integration timestep.</li> <li>- <math>t_R</math>: Relaxtion time before strething.</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>- <math>K</math>: Spring constant for the spring responsible of translating the sheet. An infinte spring constant is achieved by moving the end blocks as a rigid body (Lammps: fix move).</li> <li>- Drag Length: How far to translate the sheet.</li> <li>- Sheet size: Spatial size of the 2D sheet.</li> </ul>	Paramters that effects the simulation dynamics and the 'experimental procedure' that we a mimicking. We aim to choose to these paramters such that the friction properties is stable for small perturbations.
ML input	<ul style="list-style-type: none"> <li>- Sheet configuration: A binary matrix containing information of which atoms is removed (0) and which is still present (1) in the graphene structure.</li> <li>- Scan angle: The direction for which we translate the sheet.</li> <li>- Stretch amount: The relative sheet stretch in percentage.</li> <li>- <math>F_N</math>: Applied normal force to the end blocks.</li> </ul>	The remaining paramters that serve as the governing variables in the optimization process for certain friction properties and is thus the input variables for the ML part.

We should try to set the phycsis and measurement parameters in such a way that we reduce computation speed where it is doesn't infer with the frictional properties study.

We need to define some ranges for the ML input paramters.  $F_N$ , stretch ranges where it is not prone to ruptures. The configuration it self does not have clear rules but is also being regulated by the no rupture requirement.

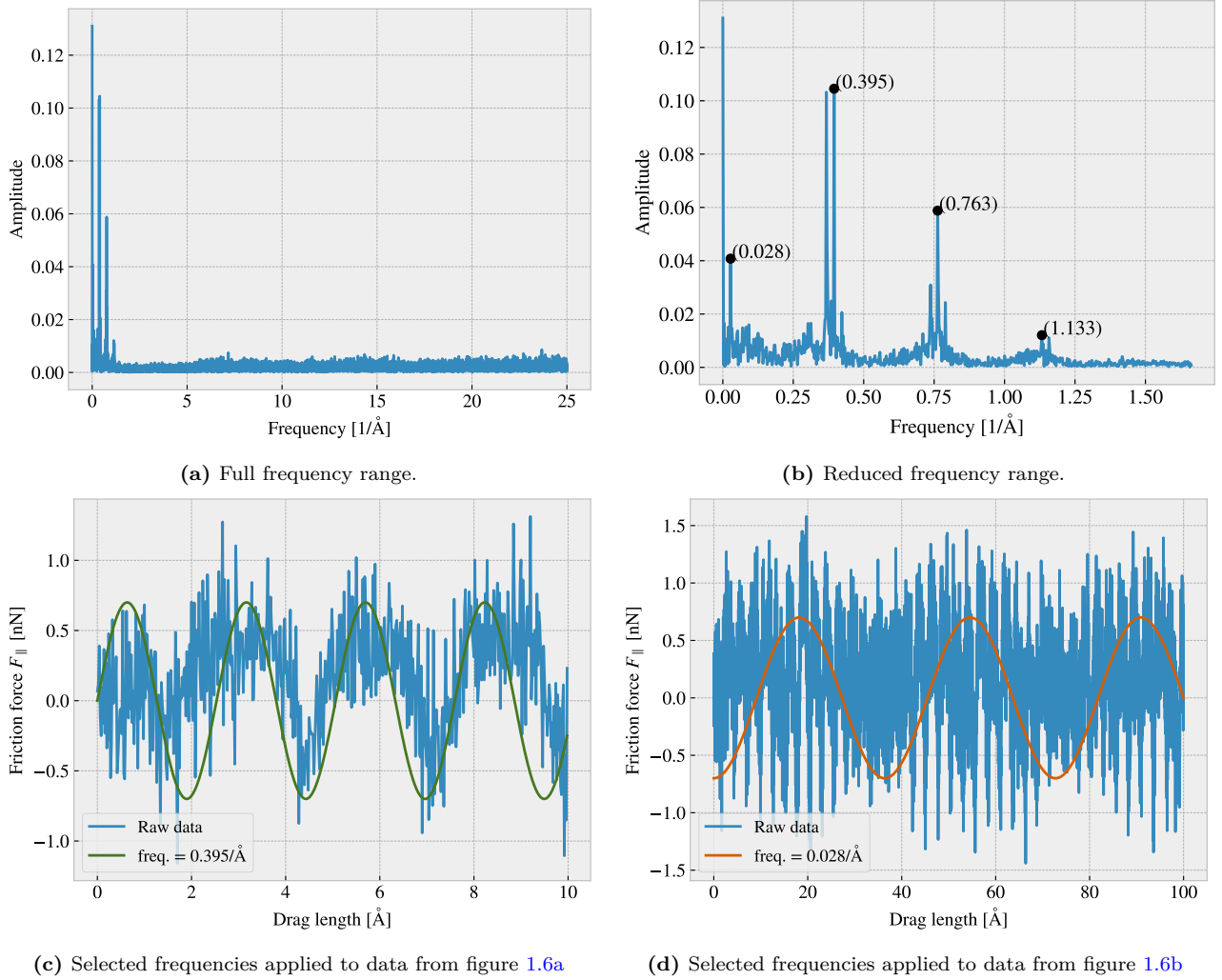
### 1.10.1 Baseline

#### 1.10.1.1 Looking at the friction data



**Figure 1.6:** Friction force  $F_{\parallel}$  between (full) sheet and substrate with respect to the drag direction vs drag length. Drag length is measured by the constant movement of the virtual atom and not the COM of the sheet. The red line represents a savgol filter with window length 150 (corresponding to a drag length of 3 Å or a time window of 15 ps) and polyorder 5.

From figure 1.6 we observe that the friction force measured parallel to the drag direction fluctuates with a wavelike pattern. By performing a fourier transform of the data we can identify some of the leading frequencies as seen in figure 1.7. We can clearly see how the frequencies of  $0.0395/\text{\AA}$  and  $0.028/\text{\AA}$  fits well with some of the slower oscillations in the data. The faster oscillations are more challenging to identify and we did not attempt to match with any sine wave here.



**Figure 1.7:** Fourier transform on data shown in figure 1.6.

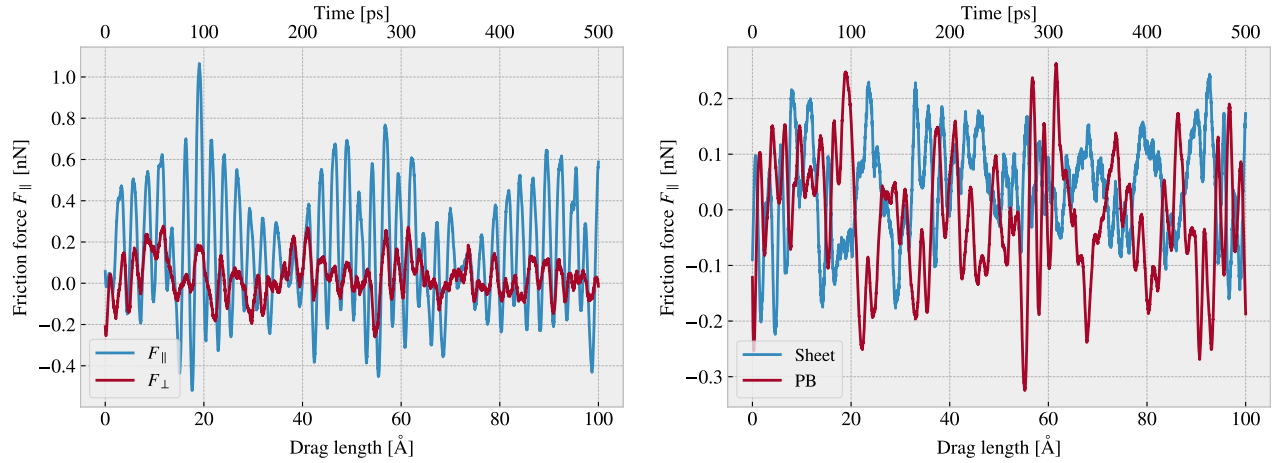
#### Decompositions.

It is tempting to only look at the friction force on the sheet since this is where we apply cuts. Any desired effect taking place here in contrast to the untouched Pull blocks can be scaled by simply increasing the size of the sheet. However as we see (in some of the figures hopefully) the distribution of force acting on the pull block and the sheet vary back and forth. Thus we cannot ignore effects of force distribution which can be induced by certain cut patterns.

What about the full sheet vs norm discussion. Are we better off just taking the full norm?

I guess the conclusion is that the para/perp decomposition show that these are easily separable + it gives a plus minus axis instead of having a friction norm. When the sheet moves backwards this should count negatively I think. For the sheet/PB decomposition we see that the pattern is not as clean when we separate them and thus we are better off keeping the full sheet measurement.

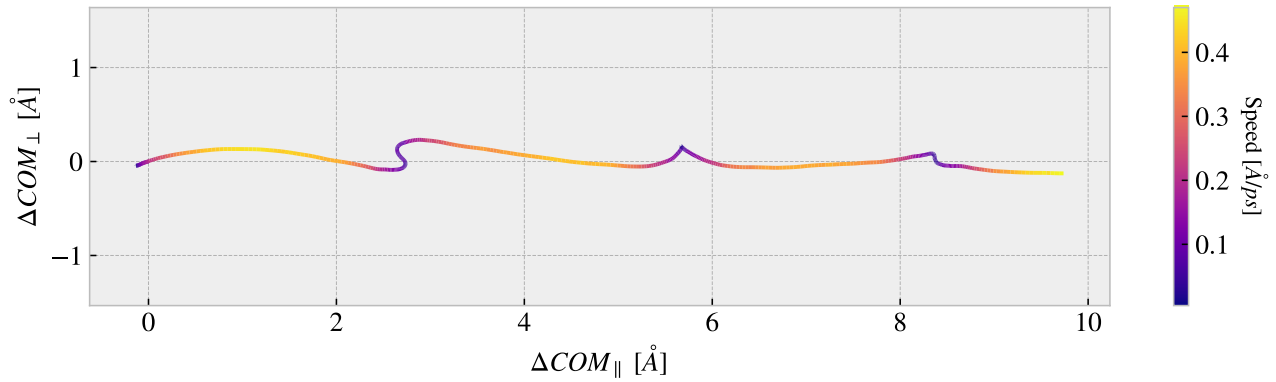




(a) Decomposition into parallel ( $\parallel$ ) and perpendicular ( $\perp$ ) to drag direction (b) Decomposition into group inner sheet (sheet) and pull blocks (PB).

**Figure 1.8:** Decomposition of friction force.

Look at the COM path.



**Figure 1.9:** ...

Should we plot some contact graphs here also? They are really not interesting until we get to the stretch part. I think we should include there as a tool for measuring the change of the sheet when stretching.

#### 1.10.1.2 Defining single metrics with uncertainty

We are interested in defining single metrics that describe the frictional properties of the sheet. A natural reference point is the dynamic and static friction coefficient. We can represent these as the mean and max friction force value respectively, but we leave the division by normal force for now as it is only a factor.

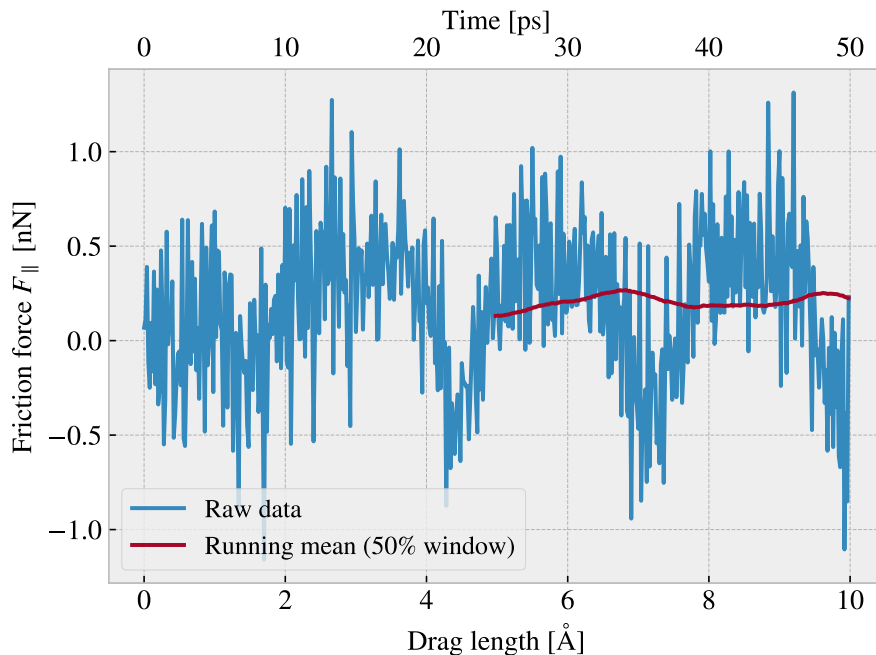
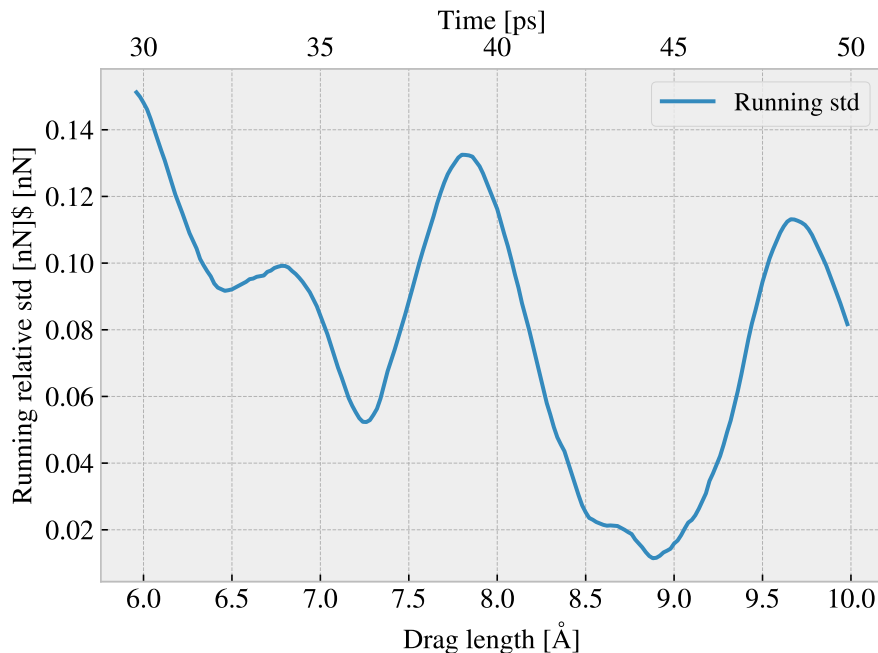


Figure 1.10: ...

A way to quantify the uncertainty of the mean friction evaluation is by looking at the running mean score shown in figure 1.10. If the running mean is constant we know that it doesn't really matter whether we stop now to measure or if we drag it a bit longer. However, any fluctuations of this line means that our mean measurement is still sensitive to the drag length. We should not care for fluctuations in the beginning of the running mean curve as this is essentially including data from the rough beginning transitioning from static to dynamic friction. Only the running mean close to the ending should be considered for our uncertainty. One way is to take the standard deviation in the final 20% of the running mean curve as a way of approximating the uncertainty of the final mean value. This is shown in figure 1.11.



**Figure 1.11:** Running std (window 20%) on runmean from figure 1.10 divided by mean of each window.

From figure 1.11 we can see that this provides us with an uncertainty at 8% relative error when stopping at drag length 10 Å. We also notice that stopping a bit earlier seemed to give better results which reflects the more stable looking part of the running mean roughly between drag length 8 Å and 9 Å. By dragging it for a total of 400 Å we get a final uncertainty of about 3.5 %. The choice of window size for these running evaluations is somewhat arbitrary and thus we should not really trust the exact numeric value of the uncertainty, but it serves as an indication of the fluctuations that we are going to pick up in our metrics which we eventually are going to pass on to neural network as true labels.

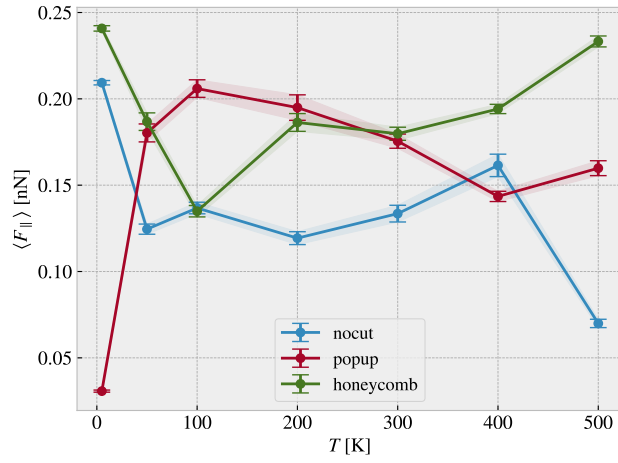
For the max value we do not really have a good way to determine the uncertainty...

### 1.10.1.3 Varying normal force and stretch

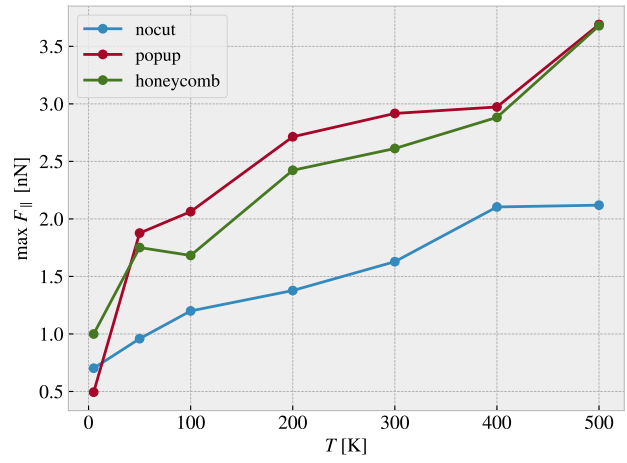
Show multi plot results with uncertainty bars.

### 1.10.1.4 (

Varying temperature, drag speed, spring constant and dt)

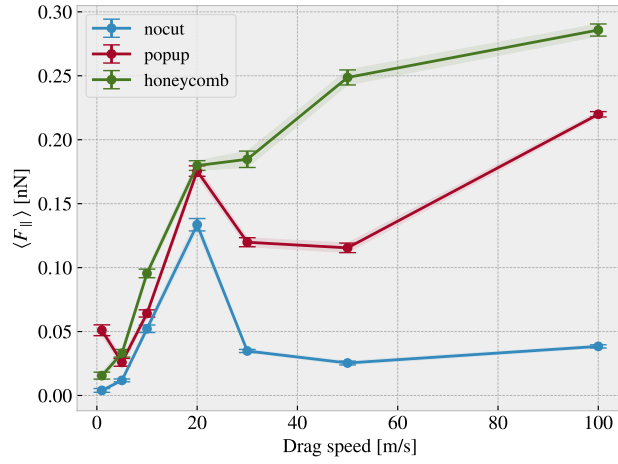


(a) mean friction

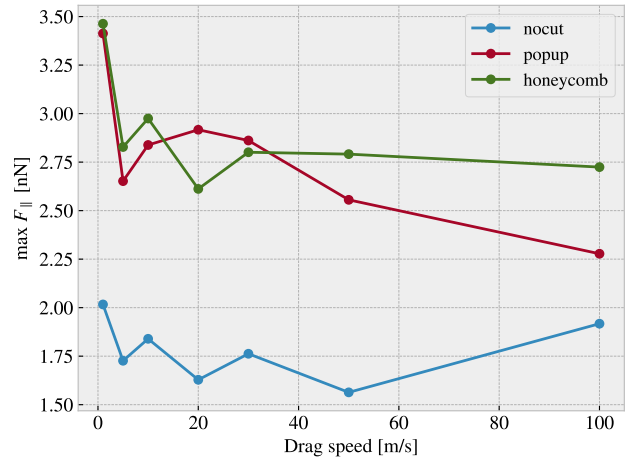


(b) max friction

Figure 1.12: Temperature

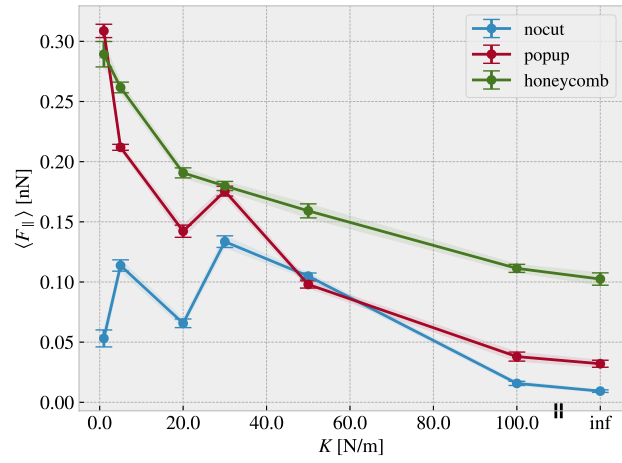


(a) mean friction

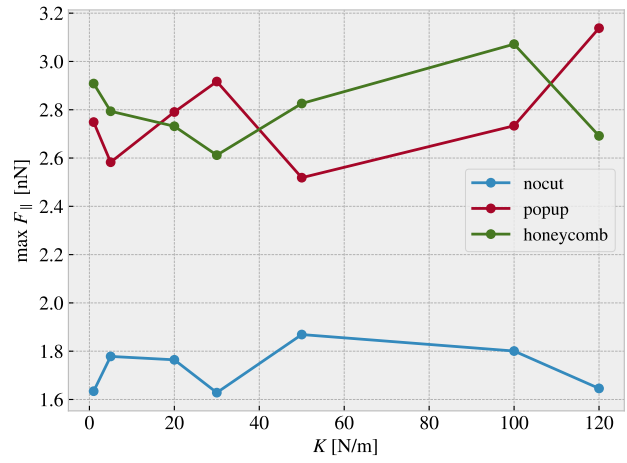


(b) max friction

Figure 1.13: Drag speed

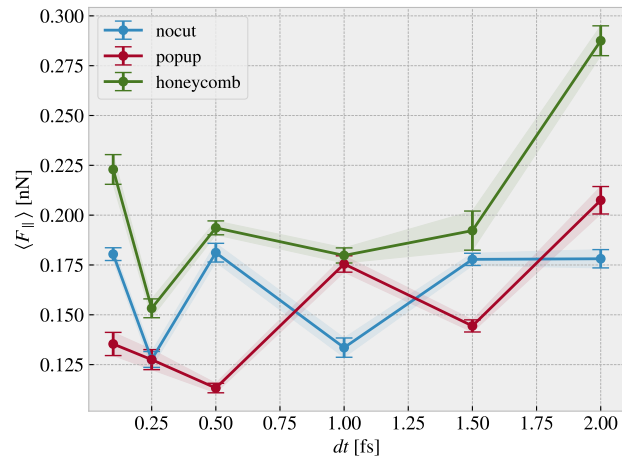


(a) mean friction

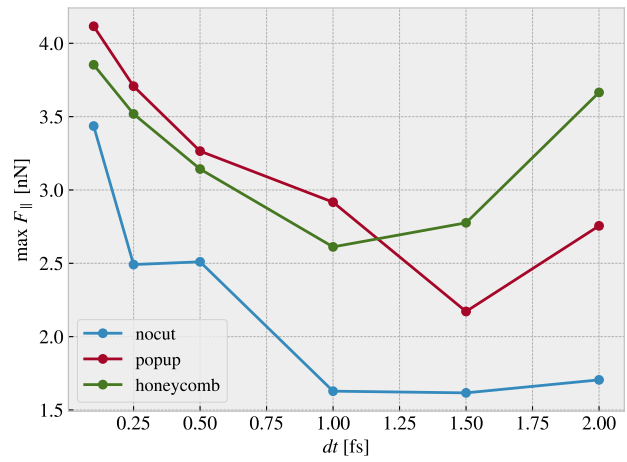


(b) max friction

Figure 1.14: Spring constant



(a) mean friction



(b) max friction

Figure 1.15: Timestep

Multi stretch

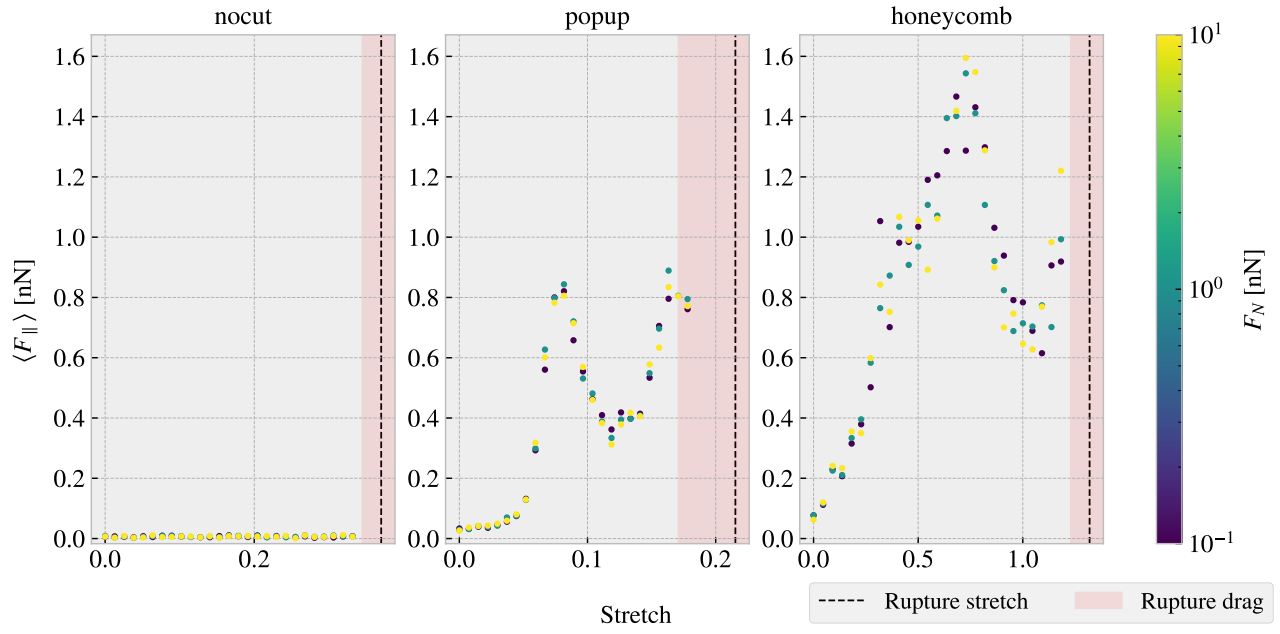


Figure 1.16: ...



Figure 1.17: ...

## Observations

- stretch = 0 % and  $F_N = 188 \text{ eV/\AA}$  yielded a very small amount of wear (two atoms visually out of place), for which the sheet dug into the substrate when passing by the second time. For the same normal force but 0.25 % this problem did not occur. We need to stay out of the friction wear regime. Amorphous substrate is even more prone to this problem of wear.





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