

Tuning Frictional Properties of Kirigami Altered Graphene Sheets using Molecular Dynamics and Machine Learning

Designing a Negative Friction Coefficient

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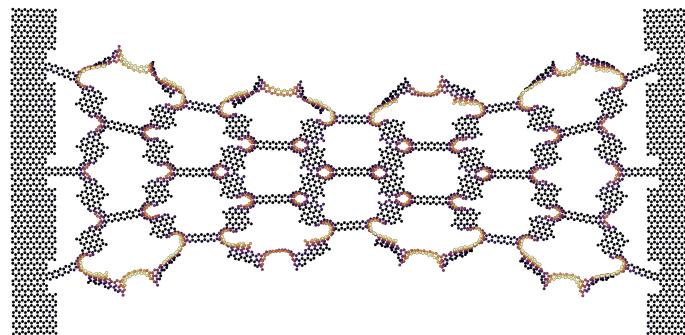
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Abstract

Abstract.

Acknowledgments

Acknowledgments.

List of Symbols

F_N Normal force (normal load)

Acronyms

MD Molecular dynamics. 2, 3

ML Machine learning. 2, 3

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Chapter 1

Introduction

Structure of Motivation section:

1. Introduce and motivate friction broadly.
2. Motives for friction control using a grasping robot as example.
3. Analog to gecko feet where adhesive properties are turned on and off.
4. Interest in origin of friction through nanoscale studies which further motivates the use of MD.
5. Intro to metamaterials and the use of kirigami designs,
6. How to optimize kirigami designs with reference to Hanakata and motivating the use of ML.
7. Out-of-plane buckling motivates the use of kirigami for frictional properties.

Does some of the latter paragraphs belong to the approach section?

1.1 Motivation

Friction is a fundamental force that takes part in most of all interactions with physical matter. Even though the everyday person might not be familiar with the term *friction* we recognize it as the inherent resistance to sliding motion. Some surfaces appear slippery and some rough, and we know intuitively that sliding down a snow covered hill is much more exciting than its grassy counterpart. Without friction, it would not be possible to walk across a flat surface, lean against the wall without falling over or secure an object by the use of nails or screws [p. 5] [1]. It is probably safe to say that the concept of friction is 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]. Today, friction is considered 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 compelling motivation to study tribology is ultimately to gain full control of friction and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages for energy efficiency. It has been reported that tribological problems have a 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].

On the other hand, the reduction of friction is not the only sensible application for tribological studies. Controlling frictional properties, besides minimization, might be of interest in the development of a grasping robot where a finetuned object handling is required. While achieving a certain “constant” friction response is readily obtained through appropriate material choices during manufacturing, we are yet to unlock the capabilities to alter friction dynamically on the go. One example from nature inspiring us to think along these lines are the gecko feet. More precisely, the Tokay gecko has received a lot of attention in scientific studies aiming to unravel the underlying

mechanism of its “toggable” adhesion properties. Although geckos are able to produce large adhesive forces, they retain the ability to remove their feet from an attachment surface at will [5]. This makes the gecko able to achieve a high adhesion on the feet when climbing a vertical surface while lifting it for the next step remains relatively effortless. For a grasping robot we might consider an analog frictional concept of a surface material that can change from slippery to rough on demand depending on specific tasks.

In the recent years an increasing amount of interest has gone into the studies of the microscopic origin of friction, due to the increased possibilities in surface preparation and the development of nanoscale experimental methods. Nano-friction is also of great concern for the field of nano-machining where the frictional properties between the tool and the workpiece dictates machining characteristics [3]. With concurrent progress in computational power and development of Molecular Dynamics (MD), numerical investigations serve as an extremely useful tool for getting insight into the nanoscale mechanics associated with friction. This simulation based approach can be considered as a “numerical experiment” enabling us to create and probe a variety of high complexity systems which are still out of reach for modern experimental methods.

In materials science such MD-based numerical studies have been used to explore the concept of so-called *metamaterials* where material compositions are designed meticulously to enhance certain physical properties [6][7][8][9][10][11]. This is often achieved either by intertwining different material types or removing certain regions completely. In recent papers by Hanakata et al. [6](2018) [7](2020) numerical studies have showcased that mechanical properties of a graphene sheet, in this case yield stress and yield strain, can be altered through the introduction of so-called *kirigami* inspired cuts into the sheet. Kirigami is a variation of origami where the paper is cut additionally to being folded. While these methods originate as an art form, aiming to produce various artistic objects, they have proven to be applicable in a wide range of fields such as optics, physics, biology, chemistry and engineering [12]. Various forms of stimuli enable direct 2D to 3D transformations through folding, bending, and twisting of microstructures. While original human designs have contributed to specific scientific applications in the past, the future of this field is highly driven by the question of how to generate new designs optimized for certain physical properties. However, the complexity of such systems and the associated design space makes for seemingly intractable problems ruling out analytic solutions.

Earlier architecture design approaches such as bioinspiration, looking at gecko feet for instance, and Edisonian, based on trial and error, generally rely on prior knowledge and an experienced designer [9]. While the Edisonian approach is certainly more feasible through numerical studies than real world experiments, the number of combinations in the design space rather quickly becomes too large for a systematic search, even when considering the simulation time on modern day hardware. However, this computational time constraint can be relaxed by the use of machine learning (ML) which have proven successful in the establishment of a mapping from the design space to physical properties of interest. This gives rise to two new styles of design approaches: One, by utilizing the prediction from a trained network we can skip the MD simulations all together resulting in an *accelerated search* of designs. This can be further improved by guiding the search accordingly to the most promising candidates, as for instance done with the *genetic algorithm* which suggest new designs based on mutation and crossing of the best candidates so far. Another, even more sophisticated approach, is through generative methods such as *Generative Adversarial Networks* (GAN). By working with a so-called *encoder-decoder* network structure, one can build a model that reverses the prediction process. That is, the model predicts a design from a set of physical target properties. In the papers by Hanakata et al. both the *accelerated search* and the *inverse design* approach was proven successful to create novel metamaterial kirigami designs with the graphene sheet.

Hanakata et al. attributes the variety in yield properties to the non-linear effects arising from the out-of-plane buckling of the sheet. Since it is generally accepted that the surface roughness is of great importance for frictional properties it can be hypothesized that the kirigami cut and stretch procedure can also be exploited for the design of frictional metamaterials. For certain designs we might hope to find a relationship between stretching of the sheet and frictional properties. If significant, this could give rise to a variability of the friction response beyond manufacturing material choice. For instance, the grasping robot might apply such a material as artificial skin for which stretching or relaxing of the surface could result in a changeable friction strength; Slippery and smooth when in contact with people and rough and firmly gripping when moving heavy objects. In addition, a possible coupling between stretch and the normal load through a nanomachine design would allow for an altered friction coefficient. This invites the idea of non-linear friction coefficients which might in theory also take on negative values given the right response from stretching. The latter would constitute an extremely rare property. This has (**only?**) been reported indirectly for bulk graphite by Deng et al. [13] where the friction kept increasing during the unloading phase. **Check for other cases and what I can really say here.**

To the best of our knowledge, kirigami has not yet been implemented to alter the frictional properties of a nanoscale system. In a recent paper by Liefferink et al. [14](2021) it is reported that macroscale kirigami can be used to dynamically control the macroscale roughness of a surface through stretching which was used to change the frictional coefficient by more than one order of magnitude. This supports the idea that kirigami designs can in fact be used to alter friction, but we believe that taking this concept to the nanoscale regime would involve a different set of underlying mechanisms and thus contribute to new insight in this field.

1.2 Approach

In this thesis we investigate the possibility to alter and control the frictional properties of a graphene sheet through application of kirigami inspired cuts and stretching of the sheet. With the use of MD simulations we evaluate the friction properties under different physical conditions in order to get insight into the prospects of this field. By evaluating variations of two kirigami inspired patterns and a series of random walk generated patterns we create a dataset containing information of the frictional properties associated with each design under different load and stretch conditions. We apply ML to the dataset and use an accelerated search approach to optimize for different properties of interest. The subtask of the thesis are presented more comprehensively in the following.

1. Define a sheet indexing that allows for a unique mapping of patterns between a hexagonal graphene lattice representation to a matrix representation suited for numerical analysis.
2. Design a MD simulation procedure to evaluate the frictional properties of a given graphene sheet under specified physical conditions such as load, stretch, temperature etc.
3. Find and implement suitable kirigami patterns which exhibit out-of-plane buckling under tensile load. This includes the creation of a framework for creating variations within each pattern class. Additionally create a procedure for generating different styles of random walk patterns.
4. Perform a pilot study of a representative subset of patterns in order to determine appropriate simulation parameters to use for the further study along with an analysis of the frictional properties shown in the subset.
5. Create a dataset consisting of the chosen kirigami variations and random walk patterns and analyse data trends.
6. Train a neural network to map from the design space to physical properties such as mean friction, maximum friction, contact area etc. and evaluate the performance.
7. Perform an accelerated search optimizing for interesting frictional properties using the ML model. This should be done both through the pattern generation procedures and by following a genetic algorithm approach.
8. Use the most promising candidates from the accelerated search to investigate the prospects of creating a nanomachine setup which exhibits a negative friction coefficient.
9. Study certain designs of interest with the scope of revealing underlying mechanism. This includes simple correlation analysis but also a visualization of feature and gradient maps of the ML network.

Is the list of subtask too specific? Some of the details here might be better suited for the thesis structure section.

1.3 Contributions

What did I actually achieve

1.4 Thesis structure

How is the thesis structured.

Part I

Background Theory

Part II

Simulations

Chapter 2

Dataset study

2.1 Generating data

The dataset consist of friction simulations of various cut configurations and combinations of normal load and stretch. For each configuration we sample 15 pseudo uniform (refer to relevant section here) strecth values between zero and the rupture stretch found in the rupture test. The normal force is uniformly sampled in the range $[0.1, 10]$ nN. In total this gives 3×15 data points for each configuration. For the remaining parameters we use the values presented in the pilot study (see ??). We generate 68 configurations of the Tetrahedron pattern type, 45 of the Honeycomb type and 100 of the Random walk type. A summary of the dataset is given in Table 2.1 while all configurations are shown explicitly in ???. Notice that not all submitted data points “makes it” to the final dataset. This is due a small variation in rupture stretch points which were not anticipated during the creation of the numerical framework for submitting multiple simulation. After performing the rupture test the simulation is restarted with a new substrate size corresponding to the measured rupture stretch limit and also with new random velocity and thermostat initializations values. The sheet is then stretched and checkpoints of the simulation state (LAMMPS restart files) are saved for each of the targeted stretch samples. However, if the rupture points arrives slightly early than syggested by the rupture test, some sampled stretch values might not get a corresponding checkpoint file. Thus, these data points are not included in the data set even though they ideally should have been noted as a rupture event. This could quite easily have been mittigated by a rewrite of that part of the code, but it was first discovered after the dataset had been created. However, the dataset still includes 11.57 % rupture events and it most likely that the most cases with a lost rupturer event have a rupture event stored for the preeceding stretch value instead which captures the information of the sheet stretch limit on its own.

Table 2.1: Summary of the number of generated data points in the dataset. Due to slight deviations in the rupture stretch and the specific numerical procedure not all submitted simulations “makes it” to the final dataset. Notice that the Tetrahedon (7, 5, 2) and Honeycomb (2, 2, 1, 5) from the pilot study is rerun as a part of the Tetrahedon and the Honeycomb datasets seperately. In the latter datasets the reference point for the pattern is randomized and thus theese configurations is not fully identical. This is the idea behind the difference of 2 in the total sum.

| Type | Configurations | Submitted data points | Final data points | Ruptures |
|-------------|----------------|-----------------------|-------------------|----------------|
| Pilot study | 3 | 270 | 261 | 25 (9.58 %) |
| Tetrahedon | 68 | 3060 | 3015 | 391 (12.97 %) |
| Honeycomb | 45 | 2025 | 1983 | 80 (4.03 %) |
| Random walk | 100 | 4500 | 4401 | 622 (14.13 %) |
| Total | 214 (216) | 9855 | 9660 | 1118 (11.57 %) |

2.2 Data analysis

In order to gain insight into the correlations between variables associated to the simulations we calculate the correlations coefficients between all variable combinations. More specific, we are going to calculate the Pearson product-moment correlation coefficient (PPMCC) for which is defined, between data set X and Y , as

$$\text{corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sigma_X \sigma_Y} = \frac{\langle (X - \mu_X)(Y - \mu_Y) \rangle}{\sigma_X \sigma_Y} \in [-1, 1]$$

where $\text{Cov}(X, Y)$ is the covariance, μ the mean value and σ the standard deviation. The correlation coefficients ranges from perfect negative correlation (-1) through no correlation (0) to a perfect positive correlation (1). The correlation coefficients is shown in Fig. 2.1

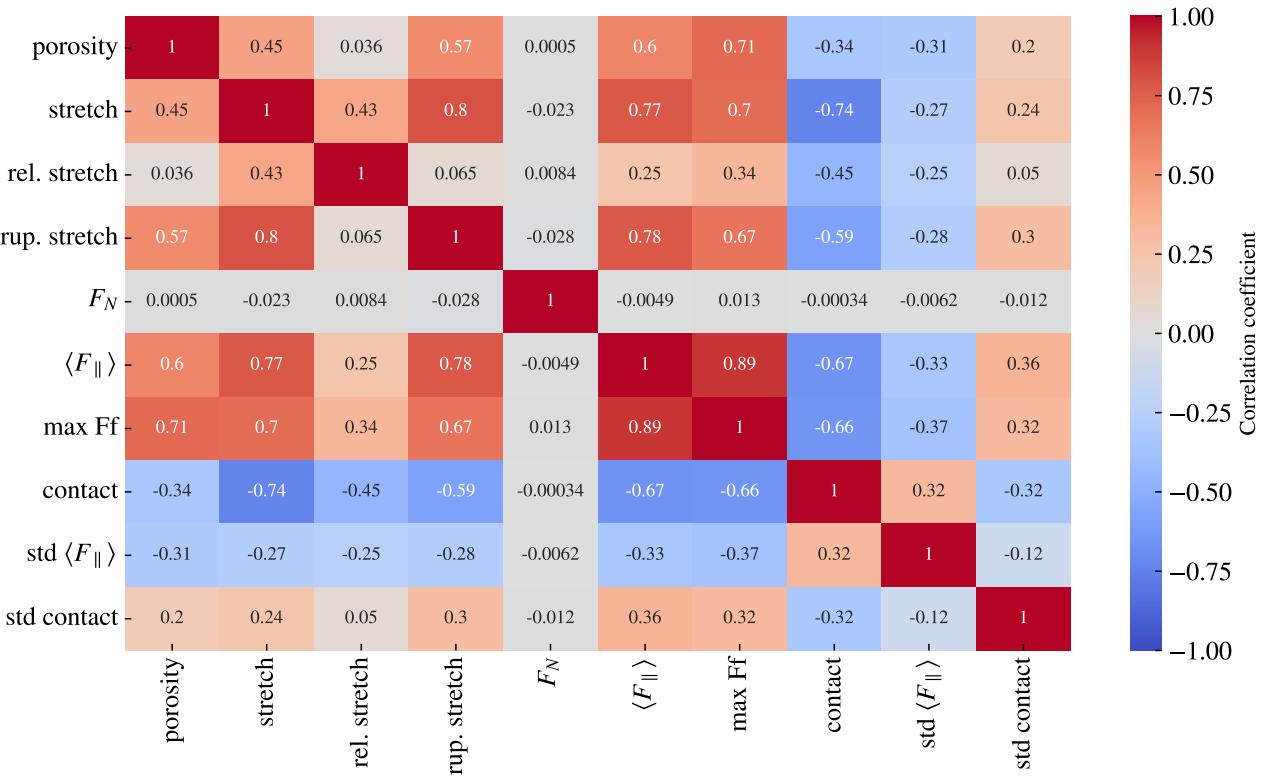


Figure 2.1: Pearson product-moment correlation coefficients for the full dataset (see Table 2.1).

From Fig. 2.1 we especially notice that the mean friction force $\langle F_{||} \rangle$ has a significant positively correlation with stretch (0.77) and porosity (0.60) (void fraction). However, the relative stretch, which is scaled by the rupture stretch, has a weaker correlation of only 0.25 which indicates that it is the absolute stretch value that has the most significant impact on the friction force increase during stretching. This is further supported by the fact that the mean friction and the rupture stretch is also strongly positively correlated (0.78). From figure Fig. 2.1 we also observe that the contact bond count is negatively correlated with the mean friction (-0.67) and the stretch value (-0.74) which is consistent with the trend observed in the pilot study ?? and ?? of the contact decreasing with increasing stretch and mean friction. However, we must take note that the correlation coefficients is a measure of the strength and slope of a forced linear fit on the data. We clearly observed a non-linear relationship between stretch and mean friction for the tetrahedron and honeycomb pattern used in the pilot study ?? where the relationship was partwise characterized by a positive correlation for some stretch ranges and partwise negative correlation for other stretch ranges. Hence, interesting strong regime-specific correlations might not be accurately highlighted by the correlation coefficients shown in Fig. 2.1.

In Fig. 2.2 we have visualized the data (excluding the pilot study) for chosen pairs of variables on the axes. In addition to a visual confirmation of how the given correlations look in a 2D plot we also get a feeling for the

coverage in various areas of the parameter space that we are eventually going to feed the neural network. The honeycomb pattern is spanning a significant larger range of stretch, contact and mean friction makes the data rather biased towards the Honeycomb pattern in those areas.

Uncommented to decrease loading time

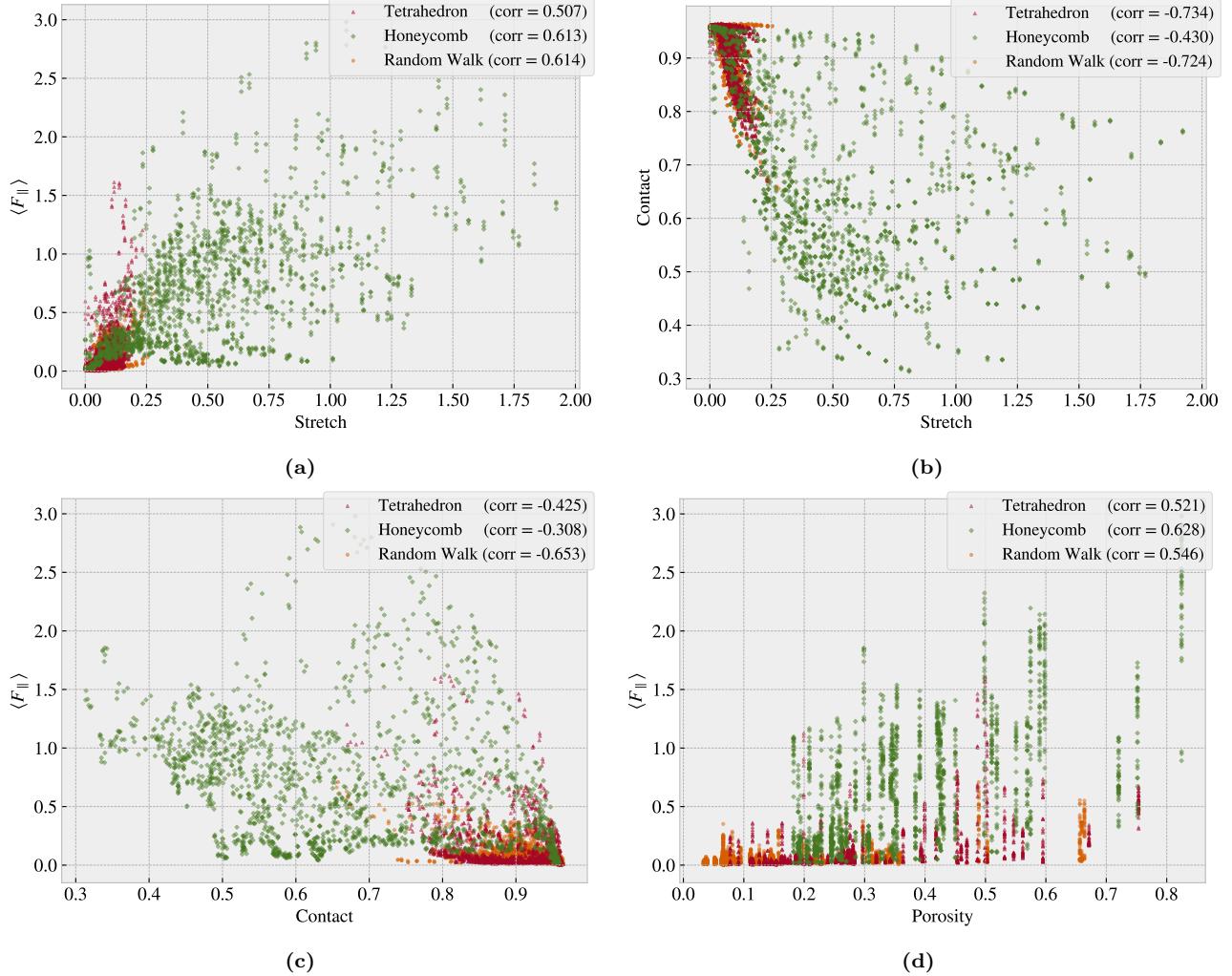


Figure 2.2: Scatter plot of the data sets Tetrahedron, Honeycomb and Random Walk (excluding the pilot study) for various variable combinations in order to visualize some chosen correlations of interest and distributions in the data

2.3 Properties of interest

From the Pilot study we discovered that it might be possible to achieve a negative friction coefficient for certain kirigami cut configurations under the assumption of a system with coupled normal force F_N and stretch S . This stands as the main property of interest to explore further in the dataset. However, it is not obvious how one should quantify this in a rigorous manner. The friction coefficient is by our definition (see theory sec XXX) given as the slope of the friction vs. normal force curve. For two data points $(F_{N,1}, F_{f,1}), (F_{N,2}, F_{f,2})$, $F_{N,1} < F_{N,2}$ we would evaluate the associated friction coefficient $\mu_{1,2}$ as

$$\mu_{1,2} = \frac{F_{f,2} - F_{f,1}}{F_{N,2} - F_{N,1}} = \frac{\Delta F_f}{\Delta F_N}$$

In the pilot study it became clear that the effects on friction under the change of F_N is negligible in comparison to the effects under change of S . Thus, by working under the assumption $F(F_N, S) \sim F(S)$ and a coupling

$F_N \propto R \cdot S$ with coupling ratio R we get

$$\mu_{1,2}(S_1, S_2) = \frac{\Delta F_f(S_1, S_2)}{R(S_2 - S_1)} \propto \frac{\Delta F_f(S_1, S_2)}{\Delta S}, \quad (2.1)$$

With the above reasoning we have in practice exchanged F_N with S in the expression for the friction coefficient. This means that we are interested in a negative slope on the friction vs. stretch curve which corresponds to a negative friction coefficient in our proposed coupled system. The next question remaining is then how to evaluate the strength of this property. By definition, the minimum slope value would give the lowest friction coefficient. However, for two data points with a small ΔS , corresponding to small denominator in Eq. (2.1), would potentially result in big $|\mu|$ without any significant decrease in friction. Hence, we choose to consider the drop in friction with increasing stretch. For a discrete dataset we can locate all local maxima and evaluate the difference to all succeeding local minima. The biggest drop will serve as our indicator for a significant negative friction coefficient. In this evaluation we do not guarantee a monotonic decrease of friction in the range of the biggest drop, but when searching among multiple configurations this is considered a descent strategy to highlight configurations of interest worthy of further investigation.

In addition to the biggest drop in friction we also look at minimum and maximum friction along with the difference between these extrema. In Table 2.2 we summarized the extrema of these properties. The corresponding friction vs. stretch profiles and configurations are visualized for each property category in Fig. 2.3 to 2.6. The stretch profiles for all the configurations are shown in appendix ??.

Table 2.2: Evaluation of the properties of interest for our dataset.

| Tetrahedron | Configuration | Stretch | Value [nN] |
|------------------------------|---------------|------------------|------------|
| Min F_{fric} | (3, 9, 4) | 0.0296 | 0.0067 |
| Max F_{fric} | (5, 3, 1) | 0.1391 | 1.5875 |
| Max ΔF_{fric} | (5, 3, 1) | [0.0239, 0.1391] | 1.5529 |
| Max drop | (5, 3, 1) | [0.1391, 0.1999] | 0.8841 |

| Honeycomb | Configuration | Stretch | Value [nN] |
|------------------------------|---------------|------------------|------------|
| Min F_{fric} | (2, 5, 1, 1) | 0.0267 | 0.0177 |
| Max F_{fric} | (2, 1, 1, 1) | 1.0654 | 2.8903 |
| Max ΔF_{fric} | (2, 1, 5, 3) | [0.0856, 1.4760] | 2.0234 |
| Max drop | (2, 3, 3, 3) | [0.5410, 1.0100] | 1.2785 |

| Random walk | Configuration | Stretch | Value [nN] |
|------------------------------|---------------|------------------|------------|
| Min F_{fric} | 12 | 0.0562 | 0.0024 |
| Max F_{fric} | 96 | 0.2375 | 0.5758 |
| Max ΔF_{fric} | 96 | [0.0364, 0.2375] | 0.5448 |
| Max drop | 01 | [0.0592, 0.1127] | 0.1818 |

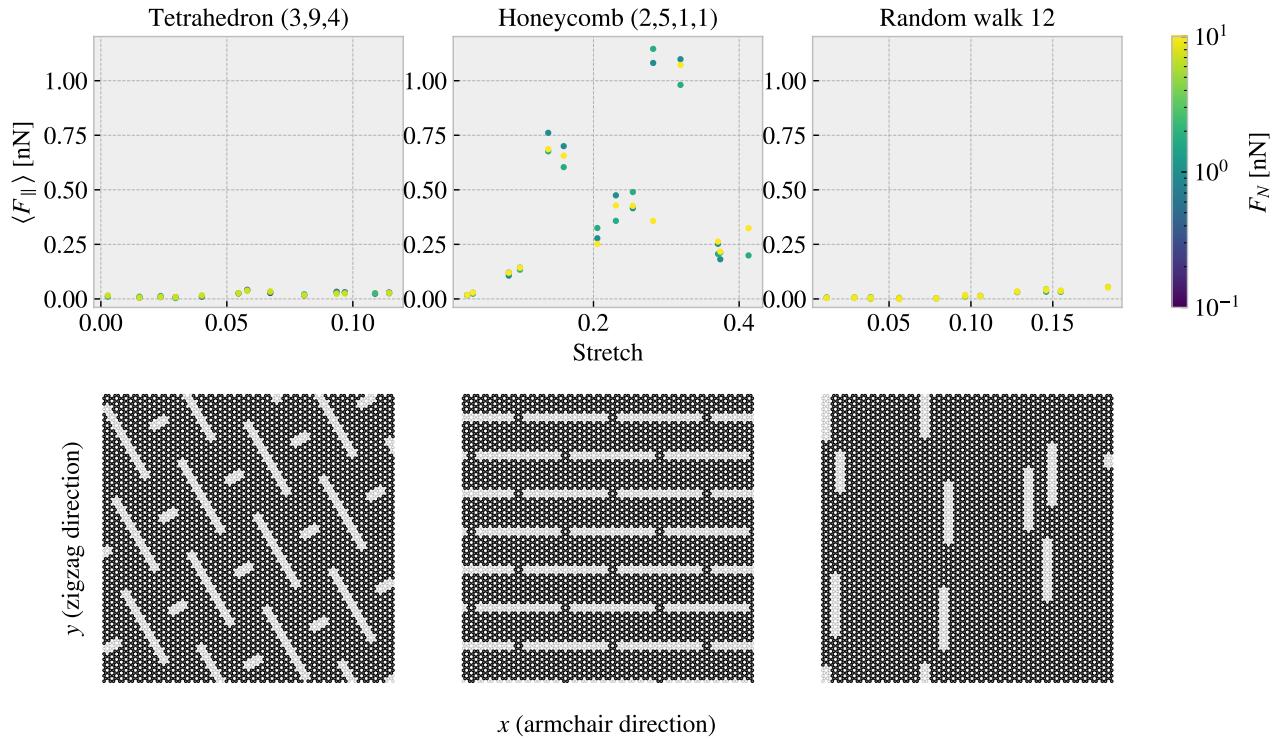


Figure 2.3: Minimum friction: Configurations corresponding to the minimum friction.

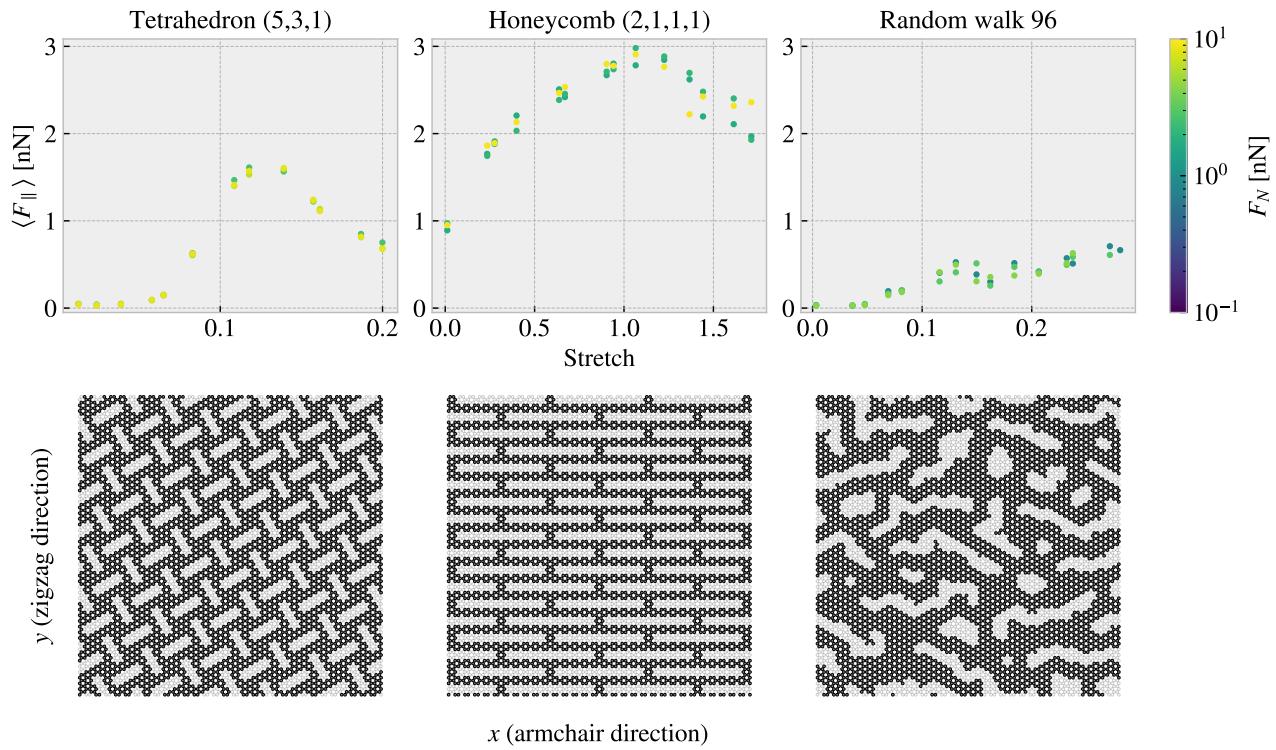


Figure 2.4: Maximum friction: Configurations corresponding to the maximum friction.

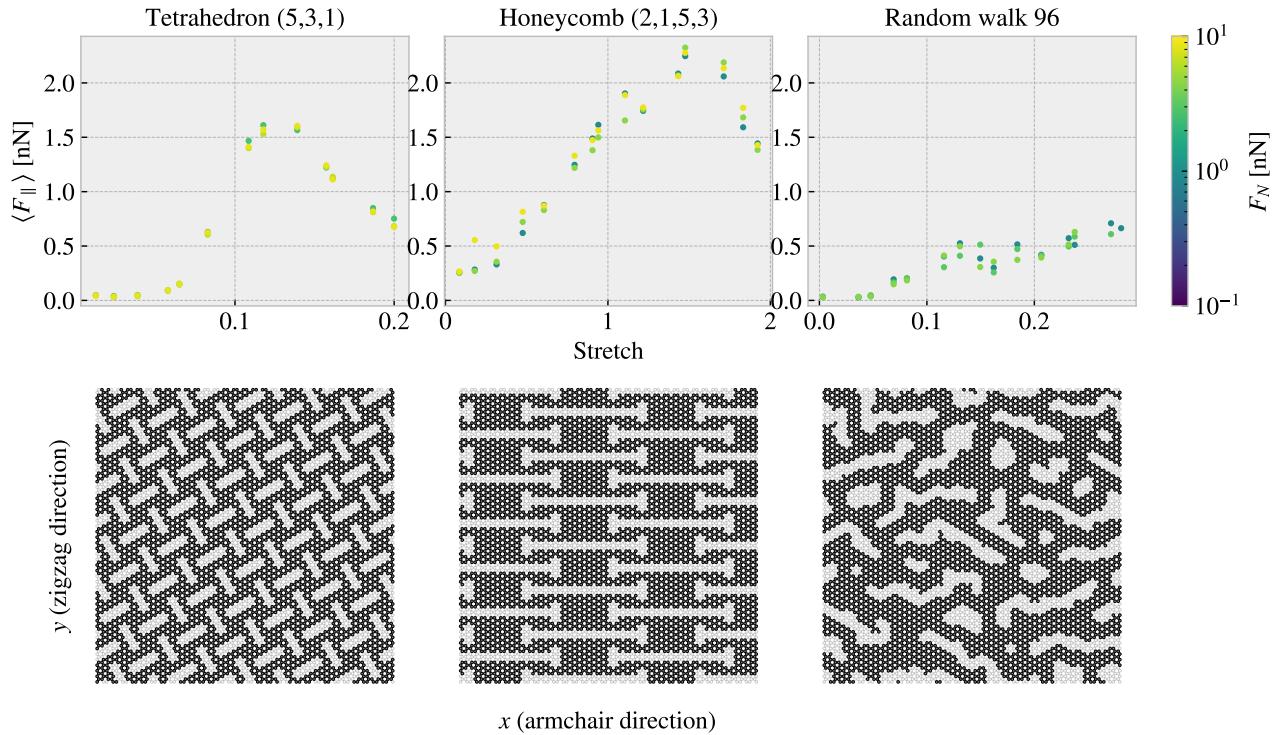


Figure 2.5: Maximum Difference: Configurations corresponding to the biggest difference in friction in the dataset for each pattern.

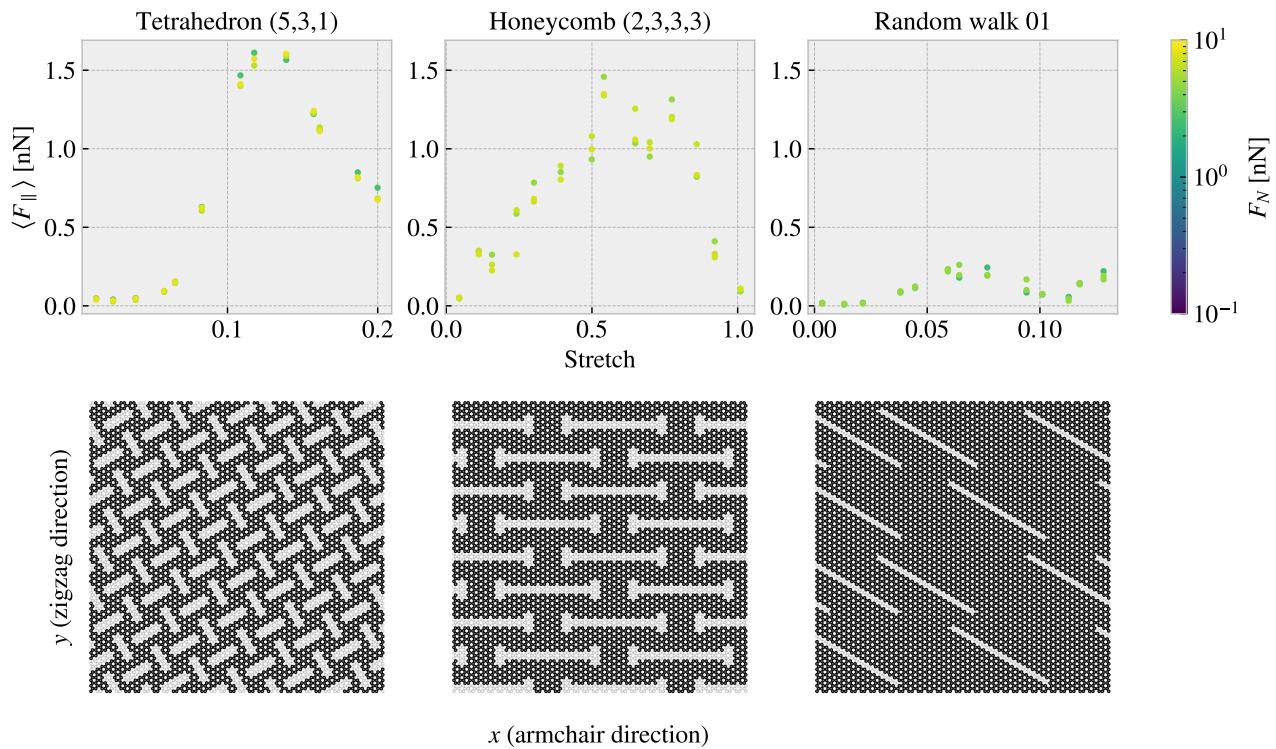
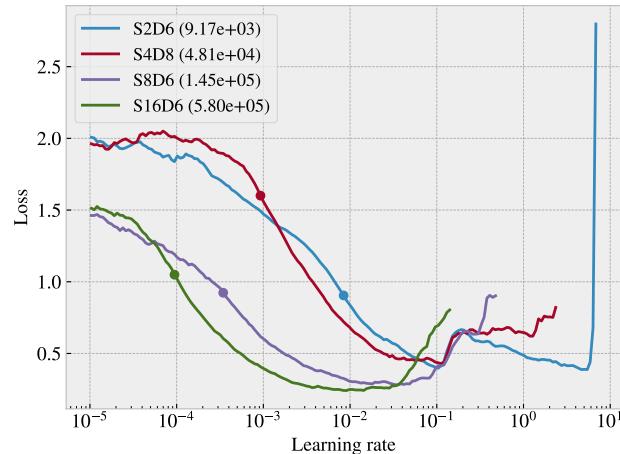


Figure 2.6: Maximum drop: Configurations corresponding to the biggest friction drop in the dataset for each pattern.

2.4 Machine learning

LR range test



(a)

Choices to make

- Learning rate: increasing LR to locate minimum in loss gradient (fastest learning) (LR range test)
- Architecture: VGGNet staircase type search
- Optimizers: Just try some different ones and look at convergence
- weight decay

Suggestion for hyperparameter tuning

1. Select complexity range of VGGNet staircase type architectures
2. Start with Adam optimizer at default settings
3. Perform LR range test to get information of a suitable LR and choose one that will work for most of the architectures.
4. Perform architecture grid search over depth and start number of channels (complexity). Choose best architecture from this.
5. Additionally add weight decay to further optimize learning for that architecture choice. Perhaps cyclic learning rates.

Start by mentioning the related articles using a VGGNet type network (and maybe also their learning rates).

Either submit with best lr for each or choose something that works for all. 0.0005 seemed as a good middle ground but the complex networks crash with these learning rates. It looks like 0.0001 (like Hanakata used) will do the job for all.

2.5 Accelerated Search

Having a network model that can predict friction force for a given configuration are able to search for some desired properties. Low and high friction and maximal negative friction coefficients

Here we pursue two different approaches for finding

1. Generate an enlarged dataset and run it through the ML model
2. Genetic algorithm

2.5.1 Markov-Chain Accelerated Genetic Algorithms

2.5.1.1 Talk about traditional method also?

2.5.1.2 Implementing for 1D chromosome (following article closely)

We have the binary population matrix $A(t)$ at time (generation) t consisting of N rows denoting chromosomes and with L columns denoting the so-called locus (fixed position on a chromosome where a particular gene or genetic marker is located, wiki). We sort the matrix rowwise by the fitness of each chromosome evaluated by a fitness function f such that $f_i(t) \leq f_k(t)$ for $i \geq k$. We assume that there are a transition probability between the current state $A(t)$ and the next state $A(t+1)$. We consider this transition probability only to take into account mutation process (mutation only updating scheme). During each generation chromosomes are sorted from most to least fitted. The chromosome at the i -th fitted place is assigned a row mutation probability $a_i(t)$ by some monotonic increasing function. This is taken to be

$$a_i(t) = \begin{cases} (i-1)/N', & i-1 < N' \\ 1, & \text{else} \end{cases}$$

for some limit N' (refer to first part of article talking about this). We use $N' = N/2$. We also define the survival probability $s_i = 1 - a_i$. In thus way a_i and s_i decide together whether to mutate to the other state (flip binary)

or to remain in the current state. We use s_i as the statistical weight for the i -th chromosome given it a weight $w_i = s_i$.

Now the column mutation. For each locus j we define the count of 0's and 1's as $C_0(j)$ and $C_1(j)$ respectively. These are normalized as

$$n_0(j, t) = \frac{C_0(j)}{C_0(j) + C_1(j)}, \quad n_1(j, t) = \frac{C_1(j)}{C_0(j) + C_1(j)}.$$

These are gathered into the vector $\mathbf{n}(j, t) = (n_0(j, t), n_1(j, t))$ which characterizes the state distribution of j -th locus. In order to direct the current population to a preferred state for locus j we look at the highest weight of row i for locus j taking the value 0 and 1 respectively.

$$\begin{aligned} C'_0(j) &= \max\{W_i | A_{ij} = 0; i = 1, \dots, N\} \\ C'_1(j) &= \max\{W_i | A_{ij} = 1; i = 1, \dots, N\} \end{aligned}$$

which is normalized again

$$n_0(j, t+1) = \frac{C'_0(j)}{C'_0(j) + C'_1(j)}, \quad n_1(j, t+1) = \frac{C'_1(j)}{C'_0(j) + C'_1(j)}.$$

The vector $\mathbf{n}(j, t+1) = (n_0(j, t+1), n_1(j, t+1))$ then provides a direction for the population to evolve against. This characterizes the target state distribution of the locus j among all the chromosomes in the next generation. We have

$$\begin{bmatrix} n_0(j, t+1) \\ n_1(j, t+1) \end{bmatrix} = \begin{bmatrix} P_{00}(j, t) & P_{10}(j, t) \\ P_{01}(j, t) & P_{11}(j, t) \end{bmatrix} \begin{bmatrix} n_0(j, t) \\ n_1(j, t) \end{bmatrix}$$

Since the probability must sum to one for the rows in the P-matrix we have

$$P_{00}(j, t) = 1 - P_{01}(j, t), \quad P_{11}(j, t) = 1 - P_{10}(j, t)$$

These conditions allow us to solve for the transition probability $P_{10}(j, t)$ in terms of the single variable $P_{00}j, t$.

$$\begin{aligned} P_{10}(j, t) &= \frac{n_0(j, t+1) - P_{00}(j, t)n_0(j, t)}{n_1(j, t)} \\ P_{01}(j, t) &= 1 - P_{00}(j, t) \\ P_{11}(j, t) &= 1 - P_{10}(j, t) \end{aligned}$$

We just need to know $P_{00}(j, t)$. We start from $P_{00}(j, t=0) = 0.5$ and then choose $P_{00}(j, t) = n_0(j, t)$

Appendices

Appendix A

Appendix B

Appendix C

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