# Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

*Designs for a negative friction coefficient.*

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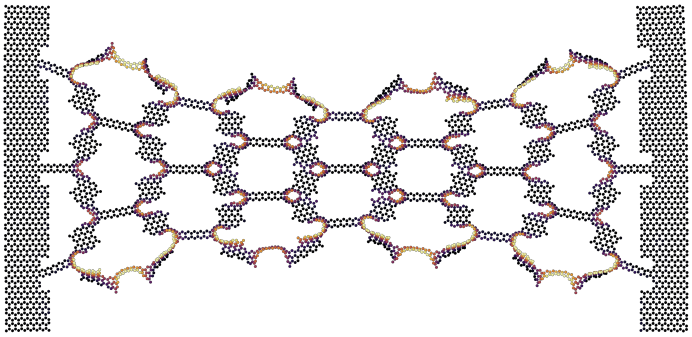

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# Abstract

Abstract.

# Acknowledgments

Acknowledgments.

# List of Symbols

$F_N$ Normal force (normal load)

# Acronyms

**GAN** Generative Adversarial Networks. 2

**MD** Molecular Dynamics. 1, 2, 3, 9, 10, 11

**ML** Machine Learning. 2, 11

# Contents

# Chapter 1

# Introduction

## 1.1 Motivation

Friction is the force that prevents the relative motion of objects in contact. 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 into our everyday life to such an extent that most people take it for granted. However, the efforts to control friction date 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 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 finetuned object handling is required. While achieving a certain "constant" friction response is readily obtained through appropriate material choices, we are yet to unlock the full 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 "togglable" adhesion properties. Although geckos can 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 them 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; Slippery and smooth when interacting with people and rough and firmly gripping when moving heavy objects.

In 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 dictate machining characteristics [3]. With concurrent progress in computational capacity and development of Molecular Dynamics (MD), numerical investigations serve as an invaluable 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 the material compositions are designed meticulously to enhance certain physical properties [6–11]. This is often achieved either by intertwining different material types or removing certain regions completely. In recent papers by Hanakata et al. [6, 7], numerical studies have showcased that the mechanical properties of a graphene sheet, 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[1] 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 computation time on modern-day hardware. However, this computational time constraint can be relaxed by the use of machine learning (ML) which has 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 altogether resulting in an *accelerated search* of designs. This can be further improved by guiding the search accordingly to the most promising candidates, for instance, as done with the *genetic algorithm* based on mutation and crossing of the best candidates so far. Another more sophisticated approach is through generative methods such as *Generative Adversarial Networks* (GAN) or diffusion models. The latter is being used in state-of-the-art AI systems such as OpenAI's DALL·E2 [13] or Midjourney [14]. By working with a so-called *encoder-decoder* network structure, one can build a model that reverses the prediction process. This is often referred to as *reverse design*, where 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. attribute the variation in mechanical 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 Kirigami-induced out-of-plane buckling can also be exploited for the design of frictional metamaterials. For certain designs, we might hope to find a relationship between the stretching of the sheet and frictional properties. If significant, this could give rise to an adjustable friction behavior beyond the point of manufacturing. 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.

In addition, the Kirigami graphene properties can be explored through a potential coupling between the stretch and the normal load, through a nanomachine design, with the aim of altering the friction coefficient. This invites the idea of non-linear friction coefficients which might in theory also take on negative values. The latter would constitute a rare property only found a few cases. These are mainly for the unloading phase of adhesive surfaces [15] or the loading phase of particular heterojunction materials [16, 17].

To the best of our knowledge, Kirigami has not yet been implemented to alter the frictional properties of a nanoscale system. However, in a recent paper by Liefferink et al. [18] it is reported that macroscale Kirigami can be used to dynamically control the macroscale roughness of a surface through stretching. They reported that the roughness change led to a changeable frictional coefficient by more than one order of magnitude. This supports the idea that Kirigami designs can be used to alter friction, but we believe that taking this concept to the nanoscale would involve a different set of governing mechanisms and thus contribute to new insight in this field.

[1] In computer science we define an *intractable* problem as a problem with no *efficient* algorithm to solve it nor any analytical solutions. The only way to solve such problems is the *brute-force* approach, simply trying all possible solutions, which is often beyond the capabilities of computational resources.

## 1.2 Goals

In this thesis, we investigate the prospects of altering the frictional properties of a graphene sheet through the application of Kirigami-inspired cuts and stretching of the sheet. With the use of molecular dynamics (MD) simulations, we evaluate the frictional properties of various Kirigami designs under different physical conditions. Based on the MD results, we investigate the possibility to use machine learning for the prediction of frictional properties and subsequently using the model for an accelerated search of new designs. The main goals of the thesis can be summarized as follows.

1. Design an MD simulation procedure to evaluate the frictional properties of a Kirigami graphene sheet under specified physical conditions.

2. Develop a numerical framework to generate various Kirigami designs, both by seeking inspiration from macroscale designs and by the use of a random walk based algorithm.

3. Investigate the frictional behavior under varying load and stretch for different Kirigami designs.

4. Develop and train a machine learning model to predict the MD simulation result and perform an accelerated search of new designs with the scope of optimizing certain frictional properties.

## 1.3 Contributions

The goals of this study [**sec:goals**]

We have discovered this and that. On the numerical side.

We have developed a numerical procedure to simulate and evaluate the frictional properties of a graphene sheet sliding on a substrate. This was done using LAMMPS [19] and might serve as useful for further studies within this topic. In addition, we have generated a framework for generating Kirigami patterns and implemented those in the simulation. This includes two classes of patterns inspired by macrscale design and a random walk algorithm for randomized designs.

What did I actually achieve Include Githib link

## 1.4 Thesis structure

In Part I: Background Theory, we cover the theoretical background related to Friction (**??**), Molecular Dynamics (**??**) and Machine Learning (**??**).

In **??**: Friction, we introduce the most relevant theoretical concepts of friction through a division by scale: Macroscale (**??**), Microscale (**??**) and nanoscale (**??**). We emphasize the nanoscale since this is of the most importance for our study. This is followed by a summary of relevant experimental and numerical results **??** and a more formal specification of our research questions (**??**).

In **??**: Molecular Dynamics, we introduce the main concepts related to the simulations used in this thesis. The main parts involve a description of the potentials used (**??**), the numerical solutions (**??**) and the modeling of temperature (**??**)

In **??**: Machine Learning, we introduce the basics of machine learning through a general presentation of the neural network **??** followed by the convolutional network (**??**) which we will use in our study. Additionally, we discuss a strategy for choosing model hypertuning (**??**) and a simple approach for model prediction explanations (). Finally, we introduce a version of the genetic algorithm applicable for accelerated search based on a machine learning model (**??**).

In Part II: Simulations, we define our numerical procedure and present and discuss the main findings of this thesis.

In **??**: System, we ...

In **??**: Pilot study, we ...

In **??**: XXX ...

In **??**: XXX, ...

The thesis is summarized in Chapter 2

Additional figures are shown in **??**, **??** and **??**. get appendix with only letter A., B. and C.

# Part I

# Background Theory

# Part II

# Simulations

# Chapter 2

# Summary

In this thesis we have studied nanoscale friction of a Kirigami graphene sheet under the influence of load and strain using MD simulations. We have developed a numerical framework for generating various Kirigami designs which was used to create a dataset of the frictional behavior depending on the Kirigami pattern, strain and loading. Our findings suggest that the frictional behavior of a Kirigami sheet is highly dependent on the geometry of the pattern and the strain conditions. We observed that the out-of-plane buckling can be associated with a non-linear friction-strain curve which can be utilized to demonstrate a negative friction coefficeint in a system with coupled load and strain. Moreover, we have investigated the possibility to use machine learning on this dataset and attempted an accelerated search. Our result suggest that machine learning can be feasible for this approach, but more data is needed to provide a more reliable foundation for a search of new Kirigami patterns. In this chapter we will summarize the findings in more detail and draw some conclusions. At the end we will provide some topics for further research.

## 2.1 Summary and conclusions

### 2.1.1 Designing an MD simulation

We have designed an MD simulation for the examination of friction for a graphene sheet sliding on a silicon substrate. The key system features were the introduction of the pull blocks, defined as the end regions of the sheet with respect to the sliding direction, which was utilized for applying normal load and sliding the sheet. The pull blocks were made partly rigid and used to employ a thermostat as well. By an analysis of the friction forces retrieved from sliding simulations we defined a standardized metric for kinetic friction. We measured the force acting from the substrate on the full sheet (including the pull blocks) with respect to the sliding direction and defined kinetic friction by the mean value of the last half of the simulation. The uncertainties were estimated on the basis of the fluctuations in the running mean. We found that the assessment of static friction was ambiguous for our simulation and did not pursue this further. From the analysis of the force traces, friction force vs. time, we identify the friction behavior in our simulation domain as being in the smooth sliding regime mainly due to the choice of sliding speed (20 m/s) and infintely stiff springs. This was further supported by a demonstration of a transition to stick-slip behavior with softer springs and a lowering of sliding speed. By conducting a more systematic investigation of the effects of temperature, sliding speed, spring constant and timestep, we settled on the default values based on numerical stability and computational cost. We found that friction increased with temperature which we attribute to being in the ballistic sliding sliding regimem. We used the room temperature 300 K as a standard choice. Furthermore, we found friction to increase with velocity as expected, with some signs of phonon resonance at certain sliding speeds as well. We chose a rather high velocity of 20 m/s mainly for the consideration of computational costs. For the spring constant, we found decreasing friction with increasing stiffness of the springs which is associated with the transition from a stick-slip-influenced regime toward smooth sliding. The choice of an infintely stiff spring was made from a stability assessment. Finally, we confirmed that a timestep of 1 fs provides reasonable numerical stability. However, based on fluctuations with timestep we find that the uncertainty in the simulations might be higher than first estimated.

### 2.1.2 Generetig Kirigami patterns

In order to invstigate the effects of Kirigami design we have created a numerical framework for generating various patterns. By defining an indexing system for the hexagonal lattice structure we were able to define the Kirigami designs as a 2D binary matrix for numerical implementation. We digitalized two different macroscale designs, which we named the *Tetrahedron* and *Honeycomb* pattern, that successfully produced out-of-plane buckling when stretched. Through our numerical framework we were able to create an ensemble of perturbed unique variations which yielded approximately 135k and 2025k for the Tetrahedron and Honeycomb patterns respectively. When considering the possibility to translate the patterns we find the ability to increase the number by roughly a factor 100. In addition we created a framework for generating random walk based Kirigami patterns. This was regulated by introducing features such as bias, avoidance of existing cuts, preference to keeping a direction and procedures to repairing the sheet for simulation purposes. In general, the capabilities of the numerical framework for generating Kirigami designs exceeded our computational resources with regard to performing MD simulation under different load and strain for each of the designs. Thus our MD-based dataset only utilized a subset of configurations with 9660 data points based on 216 Kirigami configurations (Tetrahedron: 68, Honeycomb: 45, Random walk: 100, Pilot study: 3). Thus our Kirigami generative framework can be valuable for further studies on an extended dataset.

### 2.1.3 Control friction using Kirigami

We have investigated the frictional behavior of the Tetrahedron and Honeycomb patterns in comparison to a non-cut sheet under various strains and loads. Initially, we observed that straining the Kirigami sheets in vacuum resulted in an out-of-plane buckling. When adding the substrate to the simulation this translated into a decreasing contact area with strain. We found the Honeycomb sheet to exhibit the most significant buckling with a corresponding reduction of relative contact area to approximately 43%. The non-cut sheet did not produce any significant buckling in comparison. We found that friction generally increased with strain which contradicts the asperity theory hypothesis of decreasing friction with decreasing contact area. Moreover, the friction-strain curve exhibited highly non-linear trends with strong negative slopes (see **??**), while the non-cut sheet did not show any significant dependency on the strain We also found that the non-stretched Kirigami patterns did affect friction to some degree, but this was one order of magnitude lower than the effects associated with the strain in combination. This led us to the conclusion that the changing contact area cannot be regarded as a dominant mechanism for friction in the Kirigami sheet system nor the independent consideration of sheet configuration or tension in the sheet. When considering the dependency with load we generally found a weak dependency which can be associated with a friction coefficient on the order of $10^{-4}$–$10^{-5}$ even though we could not confirm any clear relationship. This is best attributed to a superlubric state of the graphene sheet as seen in other studies as well. The slope of the friction-load curves was not considerably affected by the straining of the Kirigami sheet which led us to the conclusion that the strain-induced effects are dominant in comparison to any load-related effects. By proposing a linear coupling between load and strain with ratio $R$ we find that these results suggest the possibility to find negative friction coefficients in certain load ranges following $-R12.75\,\mathrm{nN}$ for the Tetrahedon and $-R \cdot 2.72\,\mathrm{nN}$ for the Honeycomb pattern.

### 2.1.4 Capture trends with machine learning

The dataset reveals some general correlations with mean friction, such as a positive correlation to strain (0.77) and porosity (0.60), and a negative correlation to contact area (-0.67). These results align with the finding in the pilot study, suggesting that the change in friction is associated with cuts in the sheet (porosity) and a changing contact area.

By defining the friction property metrics: $\min F_{\mathrm{fric}}$, $\max F_{\mathrm{fric}}$, $\max \Delta F_{\mathrm{fric}}$ and max drop (maximum decrease in friction with strain), we investigated the top candidates within our dataset. From these results, we found no incentive for the possibility to reduce friction with the Kirigami approach since the non-cut sheet provided the lowest overall friction. Regarding the maximum properties, we found an improvement from the original pilot study values and with the Honeycomb pattern producing the highest scores. This suggests that the data contains some relevant information for optimization with respect to these properties. Among the top candidates, we found that a flat friction-strain profile is mainly associated with little decrease in the contact area and vice versa which again aligns with the pilot study findings.

For the machine learning investigation, we have implemented a VGGNet-16-inspired convolutional neural network with a deep "stairlike" architecture: C32-C64-C128-C256-C512-C1024-D1024-D512-D256-D128-D64-D32, for convolutional layers $C$ with the number denoting channels and fully connected (dense) layers $D$ with the number denoting nodes. The final model contains $1.3 \times 10^7$ parameters and was trained using the ADAM optimizer for a cyclic learning rate and momentum scheme. We trained the network for a 1000 epochs while saving the best model during training based on the validation score. The model validation performance gives a mean friction $R^2$ score of $\sim 98\%$ and a rupture accuracy of $\sim 96\%$. However, we got lower scores for a selected subset of the Tetrahedon ($R^2 \sim 88.7\%$) and Honeycomb ($R^2 \sim 96.6$) pattern based on the top 10 max drop scores respectively. These scores were lower despite the fact that the selected set was partly included in the training data as well in addition to the fact that the hyperparameter selection favored the performance on this selected set as well. Thus we conclude that these selected configurations, associated with a highly non-linear friction-strain curve, represent a bigger challenge for the machine learning prediction. One interpretation is that these involve the most complex dynamics and perhaps that this is not readily distinguished from the behavior of the other configurations which constitute the majority of the data set. By evaluating the ability of the model to rank the dataset according to the property scores we found in general a good representation of the top 3 scores for the maximum categories, while the minimum friction property ranking was lacking. We attribute this latter observation to a higher need for precision which the model did not possess.

In order to provide a more true evaluation of the model performance we created a test set based on MD simulations for an extended Random walk search. This test revealed a significantly worse performance than seen for the validation set with a two-order of magnitude higher loss and a negative friction mean $R^2$ score which corresponds to the prediction being worse than simply guessing on the true data mean. However, by reconsidering the choice of architecture complexity hypertuning with respect to the validation loss, we found similar poor results on the test set. This indicates, that the test score is not simply a product of a biased hypertuning process but instead points to the fact that our original dataset did not cover a wide enough configuration distribution to accurately capture the full physical complexity of the Kirigami friction behavior. Based on the validation scores we conclude that the use of machine learning is feasible, but that we need to improve the dataset in order to reach a reliable model.

### 2.1.5 Accelerated search

Using the ML model we performed two types of accelerated search. One by evaluating the property scores of an extended dataset and another with the use of the genetic algorithm approach. For the extended dataset search, we used the developed pattern generators to generate $135\,\mathrm{k} \times 10$ Tetrahedon, $2025\,\mathrm{k} \times 10$ Honeycomb and $10\,\mathrm{k}$ Random walk patterns. For the minimum friction property, the search suggests a favoring of a low cut density (low porosity) which aligns with the overall idea that the dataset does not provide an incentive for further friction reduction with the non-cut sheet resulting in the lowest friction. The maximum properties resulted in some minor score increases but the suggested candidates were mainly overlapping with the original dataset. By investigating the model prediction sensitivity to the translation of the Tetrahedron and Honeycomb patterns we found that the model predictions varied drastically with small translations. This can be attributed to a physical dependency since the edge of the sheet is affected by this translation. However, due to the poor model performance on the test set, we find it more likely to be a model insufficiency related to the lacking dataset.

For the genetic algorithm approach, we investigated the optimization for the max drop property using starting population based on the result from the extended dataset accelerated search, and some random noise initializations with different porosity values. This approach did not provide any noteworthy incentive for new design structures worth more investigation. In general, the initialization of the population itself proved to be a more promising strategy than the genetic algroithm. However, this is highly affected by the uncertainty of the model predictions, and thus we did not pursue this any further. By considering the Grad-CAM explanation method we found that the model predictions occasionally payed considerable attention to the top and bottom edge of the configurations. This is surprising since these are not true edges but are connected to the pull blocks in the simulation. Despite the uncertainties in the predictions, we argue that this might be attributed to thermostat effects from the pull blocks and thus we note this as a feature worth investigating in the simulations.

### 2.1.6 Negative friction coefficient

By enforcing a coupling between load and sheet tension, mimicking a nanomachine attached to the sheet, we investigated the load curves arising from the loading of the Tetrahedron $(7, 5, 1)$ and Honeycomb $(2, 2, 1, 5)$ pattern from the pilot study. The non-linear trend observed for increasing strain carried over to the coupled system as well producing a highly non-linear friction-load curve. The Honeycomb pattern exhibited additionally a non-linear strain-tension curve which resulted in an almost discontinuous increase in friction for the initial increase in load. We attribute this feature to an unfolding process visually confirmed from the simulation frames. For the coupled system with a load-to-tension ratio of 6 we found regions in the friction-load curve with significant negative slopes. By considering the maximum and minimum points for such regions we estimated the average friction coefficient to be $-0.31$ in the range $F_N = [4.65, 6.55]$ nN for the Tetrahedron pattern and $-0.38$ in the range $F_N = [0.71, 4.31]$ nN for the Honeycomb pattern. .

Our findings suggest that the combined use of Kirigami cuts and strain has considerable potential for friction control, especially under the influence of a coupled system of load and strain.

## 2.2 Outlook

In this thesis, we have successfully shown that certain Kirigami designs exhibit non-linear behavior with strain. This discovery was done through a focus on the exploration of the effects of different designs. This invites further investigation of the underlying mechanisms behind this phenomenon. By considering one or two design, based on Tetrahedron and Honeycomb patterns, it would be valuable to investigate the effects on the friction-strain curve under various physical parameters.

First of all, we suggest an investigation of how the friction-strain curve depends on temperature, sliding speed, spring constant, and loads for an increased range $F_N > 100nN$. This is especially interesting in the context of physical conditions leading to a stick-slip behavior since our study takes a basis in smooth sliding friction. Moreover, it would be valuable to verify that the choices for relaxation time, pauses, interatomic potentials and substrate material are not critical for the qualitative observations. Especially the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential for the modeling of the graphene sheet might be of interest. In this context, it might also be useful to investigate the effects of excluding adhesion in the simulations. In order to gain further insight into the role of commensurability one could vary the scan angle as well. Since we suspect that our simulation corresponds to a incommensurable superlubric state, certain scan angles is hypothesized to yield higher friction. If the friction-strain curve is based on a commensurability effect this might yield qualitative different results and perhaps also allowing for a lowering of friction with strain. We might also consider investigating the friction-strain relationship under a uniform load to get insight into how the loading distribution effects the out-of-plane buckling and associated frictional effects.

Another topic worth studying is the relation to scale and edge effects. This includes an investigation of scaling effects, considering the ratio of the sheet to the edge, but also a translation of the sheet patterns to study the presence of any Kirigami-induced edge effects. The latter is motivated by the findings from the machine learning predictions. With this regard, we would also suggest a more detailed study of the effect of the thermostat in the pull blocks which is suggested to have a possibly importance when judging from the Grad-CAM analysis.

For the machine learning approach, our findings suggest that the dataset is extended considerably. This can be done with respect to the aim of exploring Kirigami configurations as done in this thesis, but it can also be done for a single configuration under variation of some of the simulation parameters to support some of the above mentioned investigations. In that context, one could consider more advanced model architectures and machine learning techniques. If successful this would invite further studies of inverse design methods such as GAN or diffusion models.

# Appendices

# Appendix A

# Appendix A

# Appendix A

# Appendix B

# Appendix B

# Appendix C

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