

Title

Subtitle

by

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THESIS

for the degree of

MASTER OF SCIENCE



Faculty of Mathematics and Natural Sciences  
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Title

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Title

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# Abstract

Abstract.





# Acknowledgments

Acknowledgments.



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# List of symbols?

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



# Introduction

## 0.1 Motivation

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

The most important motivation to study tribology is ultimately to gain full control of frictional and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages regarding energy efficiency. It has been reported that that monetary value of tribological problems has significant potential for economic and environmental improvements [2]:

“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.” [3].

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

In this thesis we investigate the

Friction is classically/most of the time/by default observed to increase with increasing load on the frictional surface. We know this intuitively as the fact that a heavy box is more exhausting to push across the floor than a lighter one.

With the current tribological knowledge the friction is governed positive friction coefficients. That is, the Today’s friction application is also governed by the

## 0.2 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.

### **0.3 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).

### **0.4 Contributions**

### **0.5 Thesis structure**



# Bibliography

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