Master project topics

Astrid S. de Wijn

August 27, 2018

Contents

Simulating noise generation by friction

Car brakes sometimes produce an annoying loud squealing noise. There are many other cases where noise is generated by rubbing objects together, for example in a violin. In a previous project, we have developed a simple model for studying the interplay between the dynamics at the sliding interface, and the generation of noise in a resonator such as a brake system. The goal of this project will be to further investigate this model, and study how the noise can be controlled.

The project will use a simple computational setup. As part of the project you can either use existing numerical simulations of the model or write your own. You will then expand on the old simulations. If necessary, you will run simulations on high-performance computing facilities.

This project will entail a lot of programming, and it helps if you have good understanding of mechanics. Since we already know what the model should look like, it is a fairly well-defined project.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Bjørn Haugen <bjorn.haugen@ntnu.no>

Molecular-Dynamics simulations of creep and yield in polymers exposed to water

When materials are exposed to the elements, this can speed up degredation mechanisms. In this project, you will study this by simulate bundles of polymers that are exposed to water. You will study how the water affects the elasticity and strength of the bundles by pulling them apart in different ways and surrounded with different amounts of water.

The simulations will be done in LAMMPS, a powerful molecular-dynamics package. We already have very similar simulations set up, which you can use as a basis, so this project will entail less programming than the others. However, the simulations are very time-consuming and you will need to run them on high-performance computing facilities. Because the system you will be simulating is rather complex, the data coming out of the simulations will also be quite complex. Analysing and understanding this data is where the real challenge is. It will help here if you like physics, mechanics, or materials.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Eivind Bering <eivind.bering@ntnu.no> (physics department)
Andreas Echtermeyer <andreas.echtermeyer@ntnu.no>

Building a simulation for water and diamond-like carbon coatings

Water is ubiquitous in the world around us and is present in many sliding interfaces. It is a simple molecule, but has very complex and anomalous properties. In atomistic simulations, we have quite good ways of modelling pure water. We also have good ways to model carbon and its interaction with hydrogen. However, it becomes more difficult when water starts to react with the carbon. This is problematic for our understanding and simulation of friction of carbon-based materials such as Diamond-Like Carbon (DLC) coatings and graphite under realistic conditions.

The goal of this project is to design and test a combined force field for Molecular-Dynamics (MD) simulations of DLC coatings interacting with water. You will use the simulation code LAMMPS to set up and run simulations with different force fields. The simulations will be compared to experimental results and to quantum-chemistry simulations.

Required background

A basic programming course and an interest in modelling or programming. Classical mechanics. It would help if you have taken the corrosion course or the tribology and surface technology course, but this is not strictly necessary.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

Collaborator

Sergio Armada (SINTEF)

Multiscale friction modelling for sheet metal forming: nanoscale component

The automotive industry uses Finite Element (FE) simulation to optimize forming process of automotive parts in order to reduce the cost and leas time of new vehicle programs. An accurate optimization of forming process, however, requires accurate modelling of material behaviour and contact conditions. This project is part of a joint effort with SINTEF to setup multi-scale modeling of the contact surface in forming process for the SFI Manufacturing.

The objective of this project is to use Molecular-Dynamics (MD) simulations to investigate the damage inflicted by iron tools on aluminum parts. The student will collaborate with staff/students working at different scales of the materials, where these nano-scale simulations will form an important link between DFT calculations and crystal-plasticity finite-element simulations. The students, with the support of SINTEF and NTNU staff, are requested to perform interdisciplinary work to link forming process to material physics.

Required background

Tribology or classical mechanics. A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

Collaborators

Afaf Saai and Jesper Friis (SINTEF)

Modelling extremely low friction of quasicrystals

In this project, you will focus on a particular class of crystalline materials that have an unusual structure: quasicrystals. The discovery of quasicrystals was awarded the Nobel Prize in chemistry in 2011. The project is concerned with how the quasi-crystal structure will affect the friction of these surfaces, through structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. You will write a simple numerical simulation to compute interactions of contacts with quasi-crystalline surfaces, and whenever possible do analytical calculations to accompany them.

Required background

Tribology or classical mechanics. A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

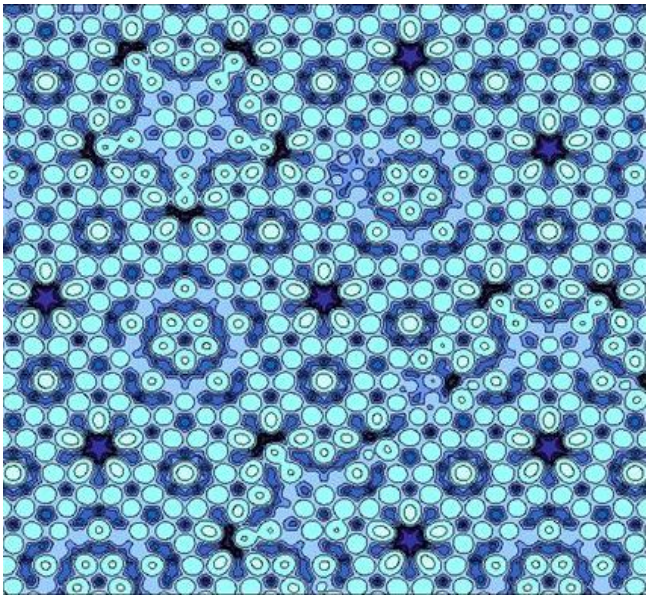

Figure 1: Example of a quasicrystal surface, atomic model of fivefold icosahedral-Al-Pd-Mn. (Picture from Wikimedia Commons.)

Simulation of a solid lubricant at the nano scale

In this project, we will investigate the mechanisms of solid lubrication using Molecular-Dynamics simulations. In lubrication with a solid powder, small, nm-thin flakes of the solid slide easily past eachother. While we have some understanding of the behaviour of single sliding flakes, we are only beginning to explore the effects of having multiple flakes that can act collectively. This project will focus on possible effects of the interactions between flakes. You will write a numerical simulation of a model for a multi-asperity contact lubricated with graphite, and run simulations.

Required background

A basic programming course and an interest in modelling or programming. Tribology, basic statistical mechanics, or classical mechanics.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

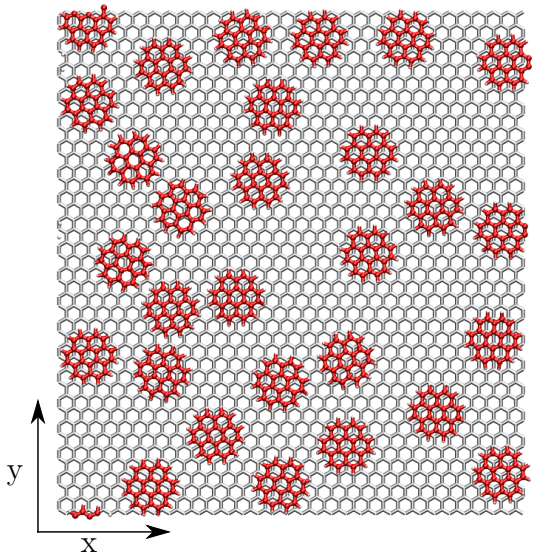

Figure 2: A top view of a simulation of a single layer of graphene flakes acting as a solid lubricant.

Molecular-Dynamics simulations of wear at the atomic scale

Wear on small scales is important not only for construction of micro and nano-scale mechanical devices (for example MEMS and NEMS), but also for understanding and preventing wear on larger scales. However, very little is understood about the mechanisms of wear at the nanometer scale.

The goal of this project is to explore different possible mechanisms by using detailed numerical simulations of a few thousand atoms and their interactions in a sliding interface. You will use the large MD code LAMMPS, combined with effective force fields, for example for iron, to simulate wear in a nano-scale contact asperity.

Required background

A basic programming course and an interest in modelling or programming. Tribology or classical mechanics.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Nuria Espallargas <nuria.espallargas@ntnu.no>

Simulation of difusion and chaos in 2d crystals

The thermodynamics or statistical physics you will have studied in your courses has all dealt with systems in equilibrium, where we have powerful formalisms. However, many interesting things happen out of equilibrium, when mass, energy, momentum, are transported. We have no powerful general theory to deal with those kinds of systems. To truly understand what is happening, we must go back to one of the fundamental assumptions: that the systems in question are chaotic.

In this project, you will investigate the connection between chaos and transport in a specific system: classical electrons or hydrogen atoms diffusing in a rigid two-dimensional crystals. We know that if the total energy is above a certain threshold, the Knauf threshold, there is always diffusion and chaos in this system. But what happens around this threshold is not clear. Is diffusion possible below the Knauf threshold? If it is, could it be anomalous? How do the diffusion and chaos relate to eachother in the vicinity of the Knauf threshold and how do they depend on the total energy? To answer these questions, you will write your own Molecular-Dynamics simulation of this system and calculate the diffusion coefficient as well as characterise the chaos.

Required background

Classical mechanics and differential equations. A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

Collaborator

Rainer Klages (Queen Mary University of London)

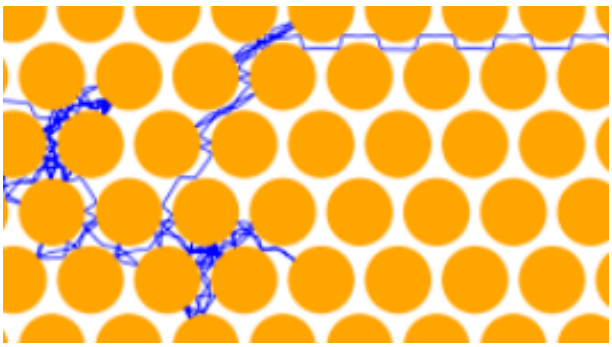

Figure 3: A section of a simulated trajectory of a classical electron in a crystal lattice. The part at the top right, where the trajectory repeats the same motion several times, is a sign that there may be anomalous diffusion.