Universität Bremen

ZARM

Master's thesis:

Simulating the effect of surface impurities on contact angle hysteresis

Wetting is a fundamental problem in fluid mechanics, with applications ranging from coating technologies to microfluidics. A key phenomenon in wetting is **contact angle hysteresis**, the difference between the advancing and receding contact angles of a liquid on a surface. While it is well understood that surface roughness and chemical heterogeneity play a major role in hysteresis, the role of *adsorbed surface impurities* remains poorly quantified. Impurities can pin the contact line, alter local surface tension, and modify force balances, yet their microscopic influence on macroscopic wetting dynamics is not fully understood.

This project will focus on **numerical simulations** of a droplet on a substrate, where impurities are modeled as localized heterogeneities with distinct wetting properties. By systematically varying impurity concentration, distribution, and strength, you will quantify their effect on advancing and receding angles, and ultimately on hysteresis. The goal is to provide a mechanistic understanding of how impurities govern droplet mobility and pinning. This work has direct relevance for industrial processes such as inkjet printing, surface cleaning, and electrolysis, as well as for natural phenomena like raindrop adhesion on leaves.

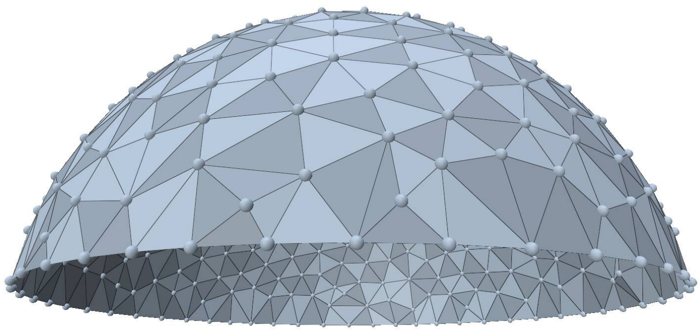

Figure 1: Triangulated droplet interface.

In this thesis, you will implement and run simulations of droplet dynamics using an existing numerical framework (github.com/Leibniz-IWT/ddgclib). You will track the motion of the three-phase contact line, measure advancing and receding angles under imposed forcing, and evaluate how impurity parameters shift the hysteresis window. If time allows, you will also compare the results to theoretical force-balance models and experimental trends from the literature.

Requirements:

- Basic knowledge of fluid mechanics and interfacial phenomena.
- Familiarity with numerical methods and coding (python preferred).
- High motivation and interest in computational physics and wetting.

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