Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Mathematical Modeling and Numerical Analysis of Transfer Processes at Dynamical Contact Lines in Fuid Mechanics

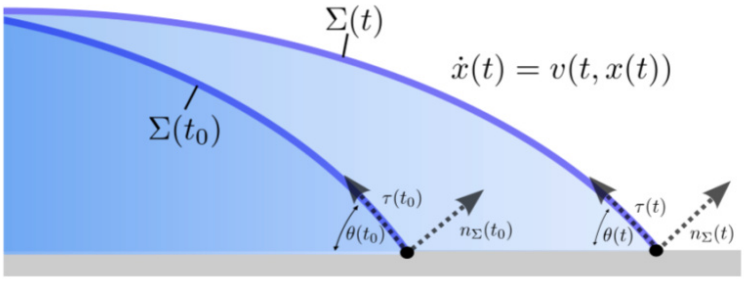


Figure1: Kinematic transport of the dynamic contact angle.

Introduction

Dynamic wetting phenomena are omnipresent in nature and technology. The legs of the water-strider make use of a sophisticated hierarchical surface structure to achieve superhydrophobicity and to allow the insect to stand and run easily on a water surface. The ability to understand and control dynamic wetting processes is crucial for a variety of industrial and technical processes such as inkjet- or bioprinting or mass transport in microfluidic devices. On the other hand, the moving contact line problem, even in a largely simplified setting, still poses considerable challenges regarding fundamental mathematical modeling as well as numerical methods.

Methods

The present work addresses both the fundamental modeling and the development of numerical methods based on the geometrical Volume-of-Fluid (VOF) method. For each control volume, we track the fraction of space occupied by each fluid. This information is used to geometrically reconstruct the interface. This geometrical representation allows us to compute the surface tension force as well as the numerical fluxes for the finite volume method.

Results

As one of the main results, we were able to prove a fundamental kinematic evolution equation describing the evolution of contact angle (i.e. the angle of intersection between the fluid-fluid interface and the solid wall) and the transporting fluid velocity field [1,2,10]. Using this tool, we also showed that physical solutions to one of the “standard models” of dynamic wetting

Project Manager
Dr. Mathis Fricke

Principal Investigator
Prof. Dr. Dieter Bothe

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Additional Software
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have to be (weakly) singular at the moving contact line. This result holds in a quite general setting and extends the knowledge about the broadly discussed “moving contact line singularity”. A compatibility analysis of the boundary conditions at the moving contact line shows that regular solutions are possible if surface mass densities are included in the modeling [1,5].

Besides the mathematical modeling, we also develop numerical methods based on both the Level Set [1,11,12] and the geometrical Volume-of-Fluid (VOF) method. In particular, we developed a novel interface reconstruction algorithm for VOF that works close to a boundary [1,3,4]. The latter method improves the accuracy of the method close to the contact line and allows for a kinematically consistent transport of the contact angle. Together with complementary numerical approaches and state-of-the-art experiments within DFG CRC 1194 and the Profile Area Thermo-Fluids & Interfaces, we are able to validate our methods in realistic test cases. In particular, we investigate the rise of liquid in a capillary tube [1,6,7,13] and the breakup of droplets on chemically patterned surfaces [1,8,9].

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