



# Numerical modelling of Super Hydrophobic Surfaces Using Lattice Boltzmann method

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## Introduction

Super Hydrophobic Surfaces (SHS) have been of interest to researchers for many years, because of their ability to reduce drag and maintain the surface to be dry and clean, and a large variety of methods have been applied to study their phenomena. The lattice Boltzmann method, thanks to its mesoscopic nature is a suitable candidate to simulate the intermolecular interactions responsible for the interfacial flows in a microscale. Additionally, the LBM is relatively easy in implementation and able to handle complex geometries such as porous media or rough surface. Computations are performed locally, thus the algorithm can be parallelized in a straightforward manner. In this contribution, we present a conservative, phase-field model for simulation of immiscible multiphase flows using an incompressible, velocity based Cascaded Lattice Boltzmann Method (CLBM). As a study case, we present a simulation of a SHS.

## How SHS works?

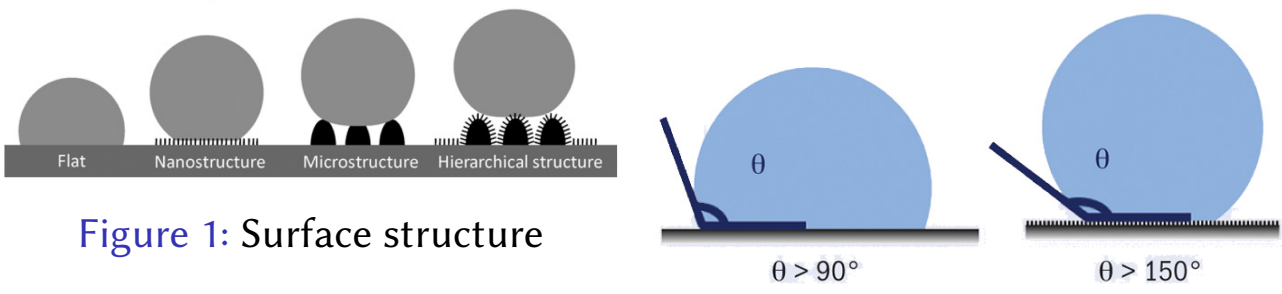


Figure 1: Surface structure

Figure 2: Coating vs structure

Generally, the super hydrophobic effect comes from both chemical interaction and surface shape in a microscale. The principle of work is based on the fact, that the tiny air-bubbles are entrapped into the microstructure of the surface being in the contact with fluids which is sliding on them. Unfortunately, usage of SHS depends on the flow condition. It may happen, that too fast flow or improper shape of the surface would cause the air-bubbles to wash out and to loose the desired properties. Chemical surface treatment can results in contact angles up to 120°. Higher values observed in a macro scale can be achieved only by additional micro roughing of the surface.

## How SHS looks like?

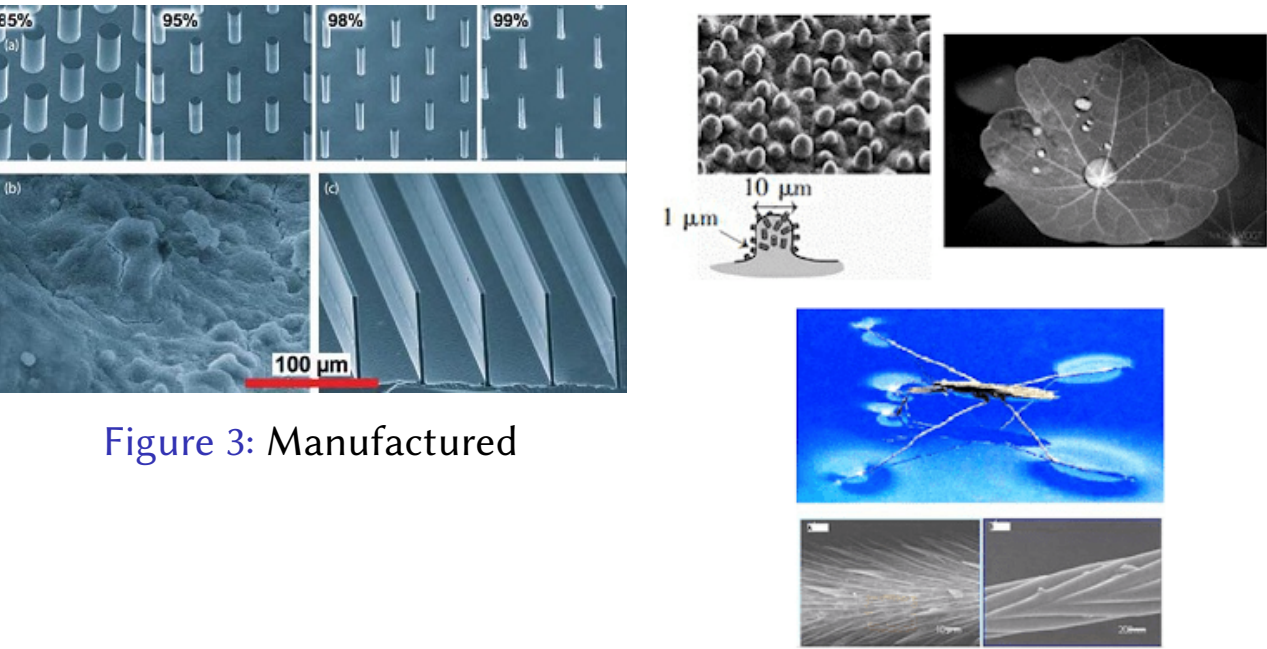


Figure 3: Manufactured

Figure 4: Natural

To support a thin layer of air, an array of posts or ridges is usually applied. Such symmetric structures are expensive to manufacture and not common in nature. However, experiments show that an unstructured rough surface can work as well as regularly spaced arrays of ridges or posts.

## Benchmarks

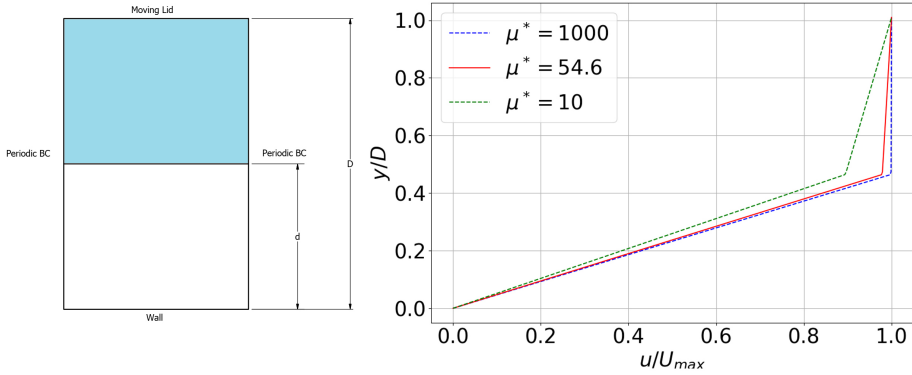


Figure 5: Two phase Couette flow:  
influence of  $\mu^*$  on velocity slip between phases

In fig. 5 we can observe that for  $\mu^* = 1000$  the velocity profile resembles a perfect slip condition. In the case of a water-air interface,  $\mu_{water-air}^* = 54.6$ , thus the common simplification of the interface by a slip BC seems to be justified with  $\sim 2\%$  error.

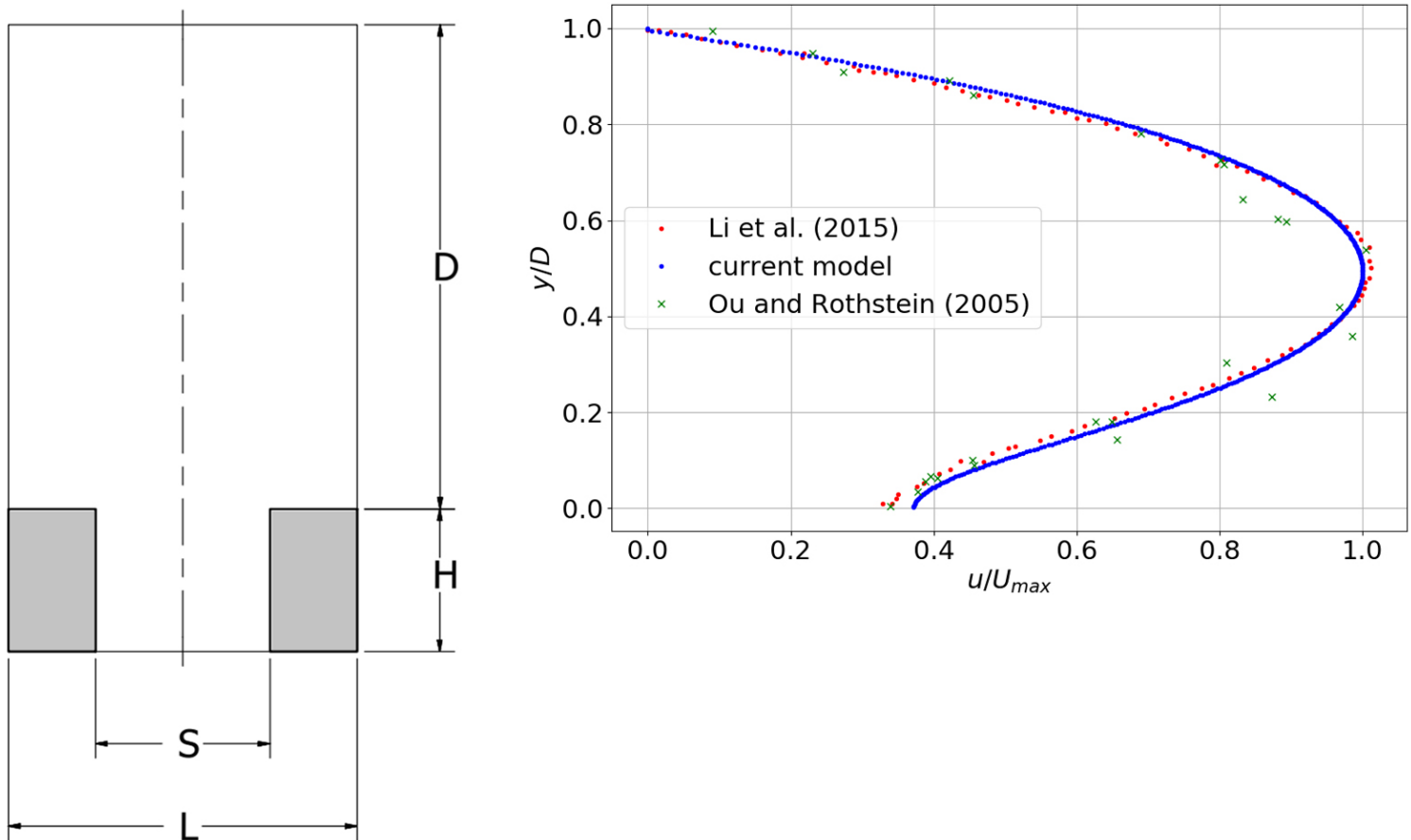


Figure 6: Dimensionless velocity profile at the center of the air pocket  $\rho^* = \mu^* = 54 : 6$

## References

Blossey, R. (2003).  
Self-cleaning surfaces - Virtual realities

## Governing Equations

We simulate an incompressible, non-miscible, multiphase flow.

The continuity and momentum equations are:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (\mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \mathbf{F}_s + \mathbf{F}_b \end{cases}$$

Forcing terms:

$$\mathbf{F}_s = \mu_\phi \nabla \phi \quad ; \quad \mathbf{F}_b = [G_x, G_y]^T$$

## Lattice Boltzmann Method

### Algorithm: hydrodynamics

1 Initialize  $\mathbf{f}(\mathbf{x}, t)$

2 Compute  $\mathbf{u} = [u_x, u_y]^T = [k_{10}, k_{01}]^T = \sum_\alpha f_\alpha \mathbf{e}_\alpha + \frac{\mathbf{F}}{2\rho} \delta t$

3 Compute

$$\tilde{\mathbf{Y}}(\mathbf{x}, t) = \mathbb{M} \mathbf{f}(\mathbf{x}, t), \quad \tilde{\mathbf{Y}}^{eq}(\mathbf{x}, t) = \dots, \quad \tilde{\mathbf{F}}(\mathbf{x}, t) = \dots$$

4 Collision

$$\tilde{\mathbf{Y}}^*(\mathbf{x}, t) = (\mathbb{I} - \mathbb{S}) \tilde{\mathbf{Y}} + \mathbb{S} \tilde{\mathbf{Y}}^{eq} + (\mathbb{I} - \mathbb{S}/2) \tilde{\mathbf{F}},$$

5 Streaming

$$\mathbf{f}(\mathbf{x} + \mathbf{e} \delta t, t + \delta t) = \mathbb{M}^{-1} \mathbb{N}^{-1} \tilde{\mathbf{Y}}^*(\mathbf{x}, t).$$

## Phase field

Interface tracking equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \phi \mathbf{u} = \nabla \cdot M \left( \nabla \phi - \frac{\nabla \phi [1 - 4(\phi - \phi_0)^2]}{|\nabla \phi| \gamma} \right)$$

Interface location:  $\phi_0 = (\phi_H + \phi_L)/2$

Density is a linear interpolation between  $\rho_H$  and  $\rho_L$ :

$$\rho = \rho_L + \frac{\phi - \phi_L}{\phi_H - \phi_L} (\rho_H - \rho_L)$$

‘Advection - Diffusion’ of  $\phi$  is solved on a separate D2Q9 lattice.

### Algorithm: phase-field

1 Initialize  $\mathbf{h}(\mathbf{x}, t)$

2 Use  $\mathbf{u}$  from hydrodynamics

3 Compute

$$\tilde{\mathbf{Y}}^\phi(\mathbf{x}, t) = \mathbb{M} \mathbf{f}(\mathbf{x}, t), \quad \tilde{\mathbf{Y}}^{\phi, eq}(\mathbf{x}, t) = \dots, \quad \tilde{\mathbf{F}}^\phi(\mathbf{x}, t) = \dots$$

4 Collision  $\tilde{\mathbf{Y}}^{\phi, *}(\mathbf{x}, t) = (\mathbb{I} - \mathbb{S}^\phi) \tilde{\mathbf{Y}}^\phi + \mathbb{S}^\phi \tilde{\mathbf{Y}}^{\phi, eq} + (\mathbb{I} - \mathbb{S}^\phi/2) \tilde{\mathbf{F}}^\phi$ .

5 Streaming

$$\mathbf{h}(\mathbf{x} + \mathbf{e} \delta t, t + \delta t) = \mathbb{M}^{-1} \mathbb{N}^{-1} \tilde{\mathbf{Y}}^{\phi, *}(\mathbf{x}, t).$$

## Summary

In this contribution, we present a conservative, phase-field model for simulation of immiscible multiphase flows using an incompressible, velocity based Cascaded Lattice Boltzmann Method (CLBM). We introduce improvements to the LB equations for interface tracking and incompressible hydrodynamics, by transforming the operations into the central moment space. The relaxation of central moments is defined in a reference frame moving with the fluid, while the previously used multiple-relaxation time scheme performs collision in a fixed reference frame. As a consequence, CLBM enhances Galilean invariance and stability of the method. As a study case, we present a simulation of a SHS.

### Treatment of an air-water interface

#### Common simplifications

- rigid surface
- perfect slip
- seek of an ideal SHS may leads to a trivial solution - two phase Couette flow

#### What we achieved

- simulations of a deformable air-water interface at micro scale
- applicable to fluids having high density ratio
- able to capture complex geometry