Lattice Boltzmann simulations in microfluidics: probing the boundary condition

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LATTICE BOLTZMANN SIMULATIONS IN MICROFLUIDICS: PROBING THE BOUNDARY CONDITION

Jens Harting · Christian Kunert · Jari Hyvälöma

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Abstract In this contribution we review our investigations of the effect of boundary slip by utilizing lattice Boltzmann simulations in order to demonstrate the applicability of the method to treat fundamental questions in microfluidics. We investigate fluid flow in hydrophobic and rough microchannels and show that a slip due to hydrophobic interactions increases with increasing hydrophobicity and is independent of the shear rate. A particular focus of the paper is on the effect of surface roughness. If surface roughness is not treated properly while analysing experimental results, a large apparent slip might be measured. We have shown that the no-slip boundary condition holds in this case if an effective surface position at an intermediate position between peaks and valleys of the surface is considered. Further, we have studied the effect of microbubbles present on a surface and shown that gas bubbles can have a strong impact on the flow properties. They can cause negative slip and due to their deformability, a shear rate dependent slip might be detected in experiments.

Keywords Apparent and intrinsic slip · rough and hydrophobic surfaces · lattice Boltzmann simulations

1 INTRODUCTION During the last few decades the miniaturization of technical devices down to submicrometric sizes has made considerable progress. In particular, during the 1980s, so-called microelectro-mechanical systems (MEMS) became available for chemical, biological and technical applications leading to the rise of a new discipline called “microfluidics” in the 1990s [1]. A wide variety of microfluidic systems was built. These include gas chromatography systems, electrophoretic separation systems, micromixers, DNA amplifiers, and chemical reactors. Next to those “practical applications”, microfluidics was used to answer fundamental questions in physics including the behavior of single molecules or particles in fluid flow or the validity of the no-slip boundary condition [1, 2]. The latter is the focus of the current review and is investigated in detail by computer simulations.

Reynolds numbers in microfluidic systems are usually small, i.e., usually below 0.1. In addition, due to the small scales of the channels, the surface to volume ratio is high causing surface effects like wettability or surface charges to be more important than in macroscopic systems. Also, the mean free path of a fluid molecule might be of the same order as the characteristic length scale of the system. For gas flows, this effect can be characterized by the so-called Knudsen number [3]. While the Knudsen number provides a good estimate for when to expect rarefaction effects in gas flows, for liquids one would naively assume that its velocity close to a surface always corresponds to the actual velocity of the surface itself. This assumption is called the no-slip boundary condition and can be counted as one of the generally accepted fundamental concepts of fluid mechanics. However, this concept was not always well accepted. Some centuries ago there were long debates about the veloc-
ity of a Newtonian liquid close to a surface and the acceptance of the no-slip boundary condition was mostly due to the fact that no experimental violations could be found, i.e., a so-called boundary slip could not be detected.

In recent years, it became possible to perform very well controlled experiments that have shown a violation of the no-slip boundary condition in sub-micron sized geometries. Since then, mostly experimental [2, 4–10], but also theoretical works [11, 12], as well as computer simulations [13–16] have been performed to improve our understanding of boundary slip. The topic is of fundamental interest because it has practical consequences in the physical and engineering sciences as well as for medical and industrial applications. Interestingly, also for gas flows, often a slip length much larger than expected from classical theory can be observed. Extensive reviews of the slip phenomenon have recently been published by Lauga et al. [2] and Neto et al. [17].

The reason for such findings is that the behavior of a fluid close to a solid interface is very complex and involves the interplay of many physical and chemical properties. These include the wettability of the solid, the shear rate or flow velocity, the bulk pressure, the surface charge, the surface roughness, as well as impurities and dissolved gas. Since all those quantities have to be determined very precisely, it is not surprising that our understanding of the phenomenon is still very unsatisfactory. Due to the large number of different parameters, a significant dispersion of the results can be observed for almost similar systems [2, 17]. For example, observed slip lengths vary between a few nanometres [18] and micrometers [5] and while some authors find a dependence of the slip on the flow velocity [4, 7, 19], others do not [5, 6].

A boundary slip is typically quantified by the so-called slip length $\beta$ – a concept that was already proposed by Navier in 1823. He introduced a boundary condition where the fluid velocity at a surface is proportional to the shear rate at the surface [20] (at $x = x_0$), i.e.,

$$v_z(x_0) = \beta \frac{\partial v_z(x)}{\partial x}. \quad (1)$$

In other words, the slip length $\beta$ can be defined as the distance from the surface where the relative flow velocity vanishes. Assuming a typical Poiseuille setup consisting of a pressure driven flow of an incompressible liquid between two infinite planes, the velocity in flow direction ($v_z$) at position $x$ between the planes is given by

$$v_z(x) = \frac{1}{2\mu} \frac{\partial P}{\partial z} \left[ d^2 - x^2 - 2d\beta \right], \quad (2)$$

where $2d$ is the distance between the planes, and $\mu$ the dynamic viscosity. $\partial P/\partial z$ is the pressure gradient. In contrast to a no-slip formulation, the last term in Eq. 2 linearly depends on the slip length $\beta$.

Most recent computer simulations apply molecular dynamics and report increasing slip with decreasing liquid density [21] or liquid-solid interactions [15], while slip decreases with increasing pressure [14]. These simulations are usually limited to a few tens of thousands of particles, length scales of a few nanometres and time scales of nanoseconds. Also, shear rates are usually some orders of magnitude higher than in any experiment [2]. Due to the small accessible time and length scales of molecular dynamics simulations, mesoscopic simulation methods such as the lattice Boltzmann method are well applicable for the simulation of microfluidic experiments.

The experimental investigation of apparent slip can be based on different setups: either a fluid is pumped through a microchannel and the measured mass flow rate at the end of the channel is compared to the theoretical value with no slip boundary conditions. From the deviation of the two values, the magnitude of slip can be computed. Another possibility is to measure the slip length directly using optical methods like particle image velocimetry (PIV). Very popular is the modification of an atomic force microscope (AFM) by adding a silicon sphere to the tip of the cantilever. While moving the sphere towards the boundary, the required force is measured. It is possible to measure the amount of slip at the wall by comparing the force needed to move the sphere with its theoretical value [10, 22].

During the last few years, the substantial scientific research invested in the slip phenomenon has lead to a more clear picture which can be summarized as follows: one can argue that many surprising results published were only due to artefacts or misinterpretation of experiments. In general, there seems to be an agreement within the community that slip lengths larger than a few nanometers can usually be referred to as “apparent slip” and are often caused by experimental artefacts. Small slip lengths are experimentally even harder to determine and require sophisticated setups such as the modified atomic force microscopes as described above. Here, small variations of the apparatus such as choosing a different shape of the cantilever or modifying the control circuit of the sample holder can lead to substantial variation of the measurements. Also, the theoretical equations correlating the measured force to the slip length are only valid for perfect surfaces and infinitely slow oscillations of the sphere. Therefore, it is of importance to perform computer simulations which have the advantage that most parameters can be changed inde-
and they do not have any obvious physical meaning. Thus, the influence of every single modification can be studied independently without modifying anything else. Therefore, they are not easily mappable to experimentally available values. We model the interaction between hydrophobic channel walls and the fluid by means of a multi-phase lattice Boltzmann model. Our approach overcomes this problem by applying a mesoscopic force between the walls and the fluid. This force can be linked to the contact angle which is commonly used by experimentalists to quantitatively describe the wettability of a material [26]. A similar approach is used by Benzi et al. [27].

The simulation method and our implementation of boundary conditions are described as follows. A multi-phase lattice Boltzmann system can be represented by a set of equations

\[
\eta_i^\alpha(x + c_i, t + 1) - \eta_i^\alpha(x, t) = \Omega_i^\alpha, \quad i = 0, 1, \ldots, b, \tag{4}
\]

where \( \eta_i^\alpha(x, t) \) is the single-particle distribution function, indicating the amount of species \( \alpha \) with velocity \( c_i \), at site \( x \) on a D-dimensional lattice of coordination number \( b \) (D3Q19 in our implementation), at time-step \( t \). This is a discretized version of equation (3) without external forces \( F \) for a number of species \( \alpha \). For the collision operator \( \Omega_i^\alpha \) we choose the Bhatnagar-Gross-Krook (BGK) form [28]

\[
\Omega_i^\alpha = -\frac{1}{\tau_\alpha}(\eta_i^\alpha(x, t) - \eta_i^\alpha eq(u^\alpha(x, t), \eta^\alpha(x, t))), \tag{5}
\]

where \( \tau_\alpha \) is the mean collision time for component \( \alpha \) and determines the kinematic viscosity

\[
\nu^\alpha = \frac{2\tau_\alpha - 1}{6}. \tag{6}
\]

of the fluid. The system relaxes to an equilibrium distribution \( \eta_i^\alpha eq \) which can be derived imposing restrictions on the microscopic processes, such as explicit mass and momentum conservation for each species. In our implementation we choose for the equilibrium distribution function

\[
\eta_i^\alpha eq = \zeta^\alpha \eta_i^\alpha \left[1 + \frac{c_i \cdot u}{c_i^2} + \frac{(c_i \cdot u)^2}{2c_i^2} - \frac{u^2}{3c_i^2} + \frac{(c_i \cdot u)^2}{6c_i^2} - \frac{u^2(c_i \cdot u)}{3c_i^4}\right], \tag{7}
\]

which is a polynomial expansion of the Maxwell distribution. \( c_i \) are the velocity vectors pointing to neighbouring lattice sites. \( c_s = 1/\sqrt{3} \) is the speed of sound for the D3Q19 lattice. The macroscopic values can be derived from the single-particle distribution function \( \eta_i^\alpha(x, t) \), i.e., the density \( \eta^\alpha(x, t) \) of the species \( \alpha \) at lattice site \( x \) is the sum over the distribution functions \( \eta_i^\alpha(x, t) \) for all lattice velocities \( c_i \),

\[
\eta^\alpha(x, t) \equiv \sum_i \eta_i^\alpha(x, t). \tag{8}
\]

\( u^\alpha(x, t) \) is the macroscopic velocity of the fluid, defined as

\[
\eta^\alpha(x, t) u^\alpha(x, t) \equiv \sum_i \eta_i^\alpha(x, t) c_i. \tag{9}
\]

2 APPARENT SLIP IN HYDROPHOBIC MICROCHANNELS

The simulation method used to study microfluidic devices has to be chosen carefully. While Navier–Stokes solvers are able to cover most problems in fluid dynamics, they lack the possibility to include the influence of molecular interactions as needed to model boundary slip. Molecular dynamics simulations (MD) are the best choice to simulate the fluid-wall interaction, but the computer power today is not sufficient to simulate length and time scales necessary to achieve orders of magnitude which are relevant for experiments. However, boundary slip with a slip length \( \beta \) of the order of many molecular diameters \( \sigma \) has been studied with molecular dynamics simulations by various authors [8,15,16,23].

In this paper we use the lattice Boltzmann method, where one discretizes the Boltzmann kinetic equation

\[
\frac{\partial}{\partial t} + v \nabla \cdot \left( \frac{x}{m} F \right) \eta(x, v, t) = \Omega(x, v, t) \tag{3}
\]

on a lattice. \( \eta(x, v, t) \) indicates the probability to find a single particle with mass \( m \), velocity \( v \) at the time \( t \) at position \( x \). The derivatives represent simple propagation of a single particle in real and velocity space whereas the collision operator \( \Omega \) takes into account molecular collisions in which a particle changes its momentum due to a collision with another particle. External forces \( F \) can be employed to implement the effect of gravity or external fields. To represent the correct physics, the collision operator should conserve mass and momentum, and should be Galilei invariant. By performing a Chapman Enskog procedure, it can be shown that such a collision operator \( \Omega \) reproduces the Navier-Stokes equation [24]. In the lattice Boltzmann method the time \( t \), the position \( x \), and the velocity \( v \) are discretized.

A few groups have applied the lattice Boltzmann method for the simulation of microlow and to study boundary slip. A popular approach is to introduce slip by generalizing the no-slip bounce back boundary conditions in order to allow specular reflections with a given probability [13]. Another possibility is to modify the fluid’s viscosity, i.e., the fluid viscosity is modified due to local density variations in order to model slip [25]. In both cases, the parameters determining the properties at the boundaries are “artificial” parameters and they do not have any obvious physical meaning.
Interactions between different fluid species are introduced following Shan and Chen as a mean field body force between nearest neighbors [29,30],

\[ \mathbf{F}^\alpha (x, t) = -\psi^\alpha (x, t) \sum_{\tilde{\alpha}} g_{\alpha \tilde{\alpha}} \sum_{\mathbf{x}'} \psi^\tilde{\alpha} (\mathbf{x}', t) (\mathbf{x}' - \mathbf{x}), \]

where \( \psi^\alpha (x, t) = (1 - e^{-\eta^\alpha (x, t)/\bar{\eta}}) \) is the so-called effective mass with \( \eta_0 \) being a reference density that is set to 1 in our case [29]. \( g_{\alpha \tilde{\alpha}} \) is a force coupling constant, whose magnitude controls the strength of the interaction between component \( \alpha \) and \( \tilde{\alpha} \). The dynamical effect of the force is realized in the BGK collision operator (5) by adding an increment \( \delta \mathbf{u}^\alpha = \tau^\alpha \mathbf{F}^\alpha / \eta^\alpha \) to the velocity \( \mathbf{u} \) in the equilibrium distribution function (7). For the potential of the wall we attach the imaginary fluid “density” \( \eta^\text{wall} \) to the first lattice site inside the wall. The only difference between \( \eta^\text{wall} \) and any other fluid packages on the lattice \( \eta^\alpha \) is that the fluid corresponding to \( \eta^\text{wall} \) is only taken into account for the collision step, but not in the propagation step. Therefore, we can adopt \( \eta^\text{wall} \) and the coupling constant \( g_{\alpha \text{wall}} \) in order to tune the fluid-wall interaction. \( g_{\alpha \text{wall}} \) is kept at 0.08 throughout this paper if not mentioned otherwise and all values are reported in lattice units. These parameters allow to simulate a wide range of effective interactions without compromising on numerical stability. Additionally, we apply second order correct mid-grid bounce back boundary conditions between the fluid and the surface [24].

From molecular dynamics simulations it is known that the fluid-wall interactions causing a slip phenomenon usually take place within a few molecular layers of the liquid along the boundary surface [8,15,16,23]. Our coarse-grained fluid wall interaction acts on the length scale of one lattice constant and does not take the molecular details into account. Therefore, our implementation is only able to reproduce an averaged effect of the interaction and we cannot fully resolve the correct flow profile very close to the wall and below the resolution of a single lattice spacing. However, in order to understand the influence of the hydrophobicity on experimentally observed apparent slip, it is fully sufficient to investigate the flow behavior on more macroscopic scales as they are accessible for experimental investigation. Our method could be improved by a direct mapping of data obtained from MD simulations to our coupling constant \( g_{\alpha \text{wall}} \) allowing a direct comparison of the influence of liquid-wall interactions on the detected slip [31].

The simulations in this work use a setup of two infinite planes separated by the distance \( 2d \). We call the direction between the two planes \( x \) and if not stated otherwise \( 2d \) is set to 64 lattice sites. In \( y \) direction we apply periodic boundary conditions. Here, 8 lattice sites are sufficient to avoid finite size effects since there is no propagation in this direction. \( z \) is the direction of the flow with our channels being 512 lattice sites long. At the beginning of the simulation \( (t = 0) \) the fluid is at rest. We then apply a pressure gradient \( \nabla P \) in the \( z \)-direction to generate a planar Poiseuille flow. Assuming Navier’s boundary condition, the slip length \( \beta \) is measured by fitting the theoretical velocity profile as given by equation 2 in flow direction \( (v_z) \) at position \( x \), to the simulated data via the slip length \( \beta \). We validate this approach by comparing the measured mass flow rate \( \int \eta v(x) dx \) to the theoretical mass flow without boundary slip and find a very good agreement. The dynamic viscosity \( \mu \) as well as the pressure gradient \( \partial P / \partial z \) needed to fit equation (2) are obtained from our simulation data.

In [31], we show that this model creates a larger slip \( \beta \) with stronger interaction, namely larger \( g_{\alpha \text{wall}} \) and larger \( \eta^\text{wall} \). The relaxation time \( \tau^\alpha \) is kept constant at 1.0 in this study and the maximum available slip length measured is 5.0 in lattice units. For stronger repulsive potentials, the density gradient at the fluid-wall interface becomes too large, causing the simulation to become unstable. At lower interactions the method is very stable and the slip length \( \beta \) is independent of the distance \( d \) between the two plates and therefore independent of the resolution. We also show that the slip decreases with increasing pressure since the relative strength of the repulsive potential compared to the bulk pressure is weaker at high pressure. Therefore, the pressure reduction near the wall is less in the high pressure case than in the low pressure one. Furthermore, we demonstrate that \( \beta \) can be fitted with a semi analytical model based on a two viscosity model.

![Fig. 1](image-url)  
**Fig. 1** Slip length \( \beta \) versus bulk velocity \( v \) for different fluid-wall interactions \( \eta^\text{wall} \). \( \beta \) is independent of \( v \) and only depends on \( \eta^\text{wall} \) [31]. All units are expressed in lattice units throughout this paper if not stated otherwise.

We study the dependence of the slip length \( \beta \) on the flow velocity for a wide range of velocities of more than three decades as it can be seen in Fig. 1 and in [31]. In the figure, we show data for different fluid-wall inter-
teractions $0 < \eta_{\text{wall}} < 2.0$ and flow velocities from $10^{-4} < v < 10^{-1}$. Within this region we confirm the findings of many steady state experiments [6], i.e., that the slip length is independent of the flow velocity and only depends on the wettability of the channel walls. Some dynamic experiments, however, find a shear rate dependent slip [19, 32]. These experiments often utilize a modified AFM as described in the introduction to detect boundary slippage. Since the slip length is found to be constant in our simulations after sufficiently long simulation times, we cannot confirm these results. However, it has been proposed by various authors that this velocity dependence is due to non-controlled effects such as impurities or surface nanobubbles.

Our mesoscopic approach is able to reach the small flow velocities of known experiments and reproduces results from experiments and other computer simulations, namely an increase of the slip with increasing liquid-solid interactions, the slip being independent of the flow velocity, and a decreasing slip with increasing bulk pressure. In addition, within our model we develop a semi-analytic approximation of the dependence of the slip on the bulk pressure as described in [31].

![Image](image.png)

**Fig. 2** A typical simulated system: Poiseuille flow between two rough surfaces showing random surface variations. Streamlines depict a two dimensional cut and illustrate the parabolic velocity profile. This profile is distorted in the vicinity of the rough surfaces [33].

The influence of surface variations on the slip length $\beta$ has been investigated by numerous authors. On the one hand roughness leads to higher drag forces and thus to no-slip on macroscopic scales. Richardson showed that even if on a rough surface a full-slip boundary condition is applied, one can determine a flow speed reduction near the boundary resulting in a macroscopic no-slip assumption [34]. Recently, we presented the idea of an effective wall for rough channel surfaces [35]. Here, we investigate the influence of different types of roughness on the position of the effective boundary. Further, we show how the effective boundary depends on the distribution of the roughness elements and how roughness and hydrophobicity interact with each other [33]. Lecoq and coworkers [36] performed experiments with well defined roughness, and developed a theory to predict the position of the effective boundary. In the experiments they utilised a laser interferometer to measure the trajectory of a colloidal sphere, and thereby determined the lubrication force and an effective boundary position. The used geometry consists of grooves with a triangular profile. For a theoretical description the boundary is expressed in a Fourier series that gives the boundary condition for the Laplace equation. From this an effective boundary can be derived by a fast converting series.

In this paper, we revise our previous achievements and compare them with the theoretical and experimental results of Lecoq and coworkers [36].

Again, Poiseuille flow measurements are utilized to investigate the effect of interest. The rough surfaces are characterised by the highest point of one plane ($h_{\text{max}}$), the position of the deepest valley ($h_{\text{min}}$) and the arithmetic average of all surface heights giving the average roughness $R_a$. In the case of symmetrical distributions we get $R_a = h_{\text{max}}/2$.

The position of the effective boundary $h_{\text{eff}}$ can be found by fitting the parabolic flow profile via the distance $2d = 2d_{\text{eff}}$. With $\beta$ set to 0 we obtain the no-slip case. To obtain an average value for the effective distance between the planes $d_{\text{eff}}$, a sufficient number of individual profiles at different positions $z$ are taken into account. The so found $d_{\text{eff}}$ gives the position of the effective boundary and the effective height $h_{\text{eff}}$ of the rough surface is then defined by $d_{\text{max}} - d_{\text{eff}}$.

We show that the position of the effective boundary height is depending on the shape of the roughness elements, i.e., for strong surface distortions it is between 1.69 and 1.90 times the average height of the roughness $R_a = h_{\text{max}}/2$ [35]. In Fig 3 we plot the effective boundary positions of different geometries, i.e. randomly distributed grooves with a square profile and grooves with a triangular profile. The results for the triangular ones...
match with the theoretical value of Lecoq et al. [36] for a similar geometry.

![Figure 3](image1.png)

**Fig. 3** Simulated effective height $h_{eff}$ versus $R_a$ for different surface geometries. The triangular shape matches the theoretical results of Lecoq et al. [36] for a similar geometry.

By adding an additional distance between roughness elements, $h_{eff}$ decreases slowly, so that the maximum height is still the leading parameter. We are also able to simulate flow over surfaces generated from AFM data of gold coated glass used in microflow experiments by O.I. Vinogradova and G.E. Yakubov [37]. We find that the height distribution of such a surface is Gaussian and that a randomly arranged surface with a similar distribution gives the same result for the position of the effective boundary although in this case the heights are not correlated.

![Figure 4](image2.png)

**Fig. 4** Simulated effective height $h_{eff}$ versus $R_a$ for gold coated glass surfaces and a randomly generated surface with Gaussian distributed heights. The background image shows the gold surface on the left and the artificially generated structure on the right [35].

We can tune the width of the distribution $\sigma$ and the average height $R_a$. By scaling $\sigma$ with $R_a$ we obtain geometrically similar geometries. This similarity is important because the effective height $h_{eff}$ scales with the average roughness in the case of geometrical similarity [35]. We investigate Gaussian distributed heights with different widths $\sigma$ and find that the height of the effective wall depends linearly on $\sigma$ in the observed range [33]. Further, we find that the slip diverges as the amplitude of the roughness increases and the flow field gets more restricted which highlights the importance of a proper treatment of surface variations in very confined geometries [35].

### 4 STRUCTURED SURFACES WITH ENTRAPPED MICROBUBBLES

A natural continuation of our previous works on roughness induced apparent boundary slip and the collaboration mentioned above is the analysis of flow along superhydrophobic surfaces [38]. While in typical experiments, slip lengths of a few tens of nanometers can be observed, it would be preferable for technical applications to increase the throughput of fluid in a microchannel, i.e., to obtain substantially larger slip. Superhydrophobic surfaces are promising in this context, since it has been recently predicted [39] and experimentally reported [40] that the so-called Fakir effect or Cassie state considerably amplifies boundary slippage. Using highly rough hydrophobic surfaces such a situation can be achieved. Instead of entering the area between the rough surface elements, the liquid remains at the top of the roughness and traps air in the interstices. Thus, a very small liquid-solid contact area is generated.

Steinberger et al. utilized surfaces patterned with a square array of cylindrical holes to demonstrate that gas bubbles present in the holes may cause a reduced slip [41]. Numerically, they found even negative slip lengths for flow over such bubble mattresses, i.e., the effective no-slip plane is inside the channel and the bubbles increase the flow resistance. In this section we consider negative slip lengths on bubble surfaces and also discuss the question of shear-rate dependent slip. In particular we show that microbubbles can generate a shear-rate dependence.

Our simulations utilize the single component multiphase LB model by Shan and Chen [30] which enables simulations of liquid-vapor systems with surface tension. The flow is confined between two parallel walls. One of the walls is patterned with holes and vapor bubbles are trapped to these holes. The other wall is smooth and moved with velocity $u_0$. Steinberger et al. [41] presented finite-element simulations of flow over rigid “bubbles” by applying slip boundaries at static bubble surfaces. The LB method allows the bubbles to deform if the viscous forces are high enough compared to the surface tension. We are also interested in how surface pat-
tering affects the slip properties of these surfaces, and how bubbles could be utilized to develop surfaces with special properties for microfluidic applications [38].

![Image 5](image_url)

**Fig. 5** A visualisation of the simulation setup (left): the lower surface is patterned with holes, while the upper surface is moved with velocity \( u_0 \). Right: the slip length \( \beta \) as a function of protrusion angle \( \varphi \). A unit cell of each array is shown in insets and corresponding results are given by triangles (rhombic array), diamonds (rectangular array), and circles (square array). The inset in the top-left corner shows the definition of \( \varphi \) [38].

The distance between walls is \( d = 1 \, \mu\text{m} \) (40 lattice nodes) in all simulations, and the area fraction of holes is 0.43. A unit cell of the regular array is included in a simulation and periodic boundary condition are applied at domain boundaries. The bubbles are trapped to holes by using different wettabilities for boundaries in contact with the main channel and with the hole. The protrusion angle \( \varphi \) (see Fig. 5 for definition) is varied by changing the liquid’s bulk pressure. The effective slip length is \( \beta = \mu u_0/\sigma - d \), where \( \sigma = \mu d v/\Delta z \) is the shear stress acting on the upper wall and \( \mu \) the dynamic viscosity of the liquid.

We investigate the effect of a modified protrusion angle and different surface patterns by using square, rectangular, and rhombic bubble arrays. The cylindrical holes have a radius \( a = 500 \, \text{nm} \) and the area fraction of the holes is equal in all cases. The shear rate is such that the Capillary number \( Ca = \mu a G_s/\gamma = 0.16 \). Here, \( G_s \) and \( \gamma \) are the shear rate and surface tension, respectively. A snapshot of a simulation is shown in the left part of Fig. 5 and the slip lengths obtained are shown in the right part. The observed behavior is similar to that reported in [41], where a square array of holes was studied. In particular, we observe that when \( \varphi \) is large enough \( \beta \) becomes negative. Moreover, when the protrusion angle equals zero, the slip length is maximised and the highest possible throughput in a microchannel is obtained. The behavior of the slip length can be explained by thinking of an increased surface roughness if the protrusion angle is larger or smaller than zero. Since the area fraction of the bubbles is the same in all three cases, our results clearly indicate that slip properties of the surface can be tailored not only by changing the protrusion angle but also by the array geometry. In the presented study, the highest slip lengths are obtained for the rhombic unit cell and it is current work of progress to investigate the influence of the array geometry in more detail.

Next, the shear-rate dependence of the slip length is investigated. As the shear rate and thus the viscous stresses grow the bubbles are deformed (see Fig. 6, left) and the flow field is modified. In the central part of Fig. 6, we show the simulated slip length as a function of the Capillary number for three different protrusion angles. The Capillary numbers chosen are in higher end of the experimentally available range. Our results show shear-rate dependent slip, but the behavior is opposite to that found in some experiments: in fact, the slip lengths measured by us decrease with increasing shear due to a deformation of the bubbles. In the experiments, surface force apparatuses are used (see, e.g., Ref. [19]), where a strong increase in the slip is observed after some critical shear rate. This shear-rate dependence has been explained, e.g., with formation and growth of bubbles [12, 42]. In our simulations, there is no formation or growth of the bubbles as we only simulate a steady case for given bubbles. The experiments on the other hand are dynamic. However, our results indicate that the changes in the flow field which occur due to the deformation of the bubbles cannot be an explanation for the shear-rate dependence observed in some experiments. Our results are consistent with [35] and the previous section, where it is shown that smaller roughness leads to smaller values of a detected slip. In the present case, the shear reduces the average height of the bubbles and thus the average scale of the roughness decreases as well.

Finally, we consider a surface patterned with grooves. Cylindrical bubbles protrude to the flow channel from these holes with protrusion angle \( \varphi = 72^\circ \), and the area fraction of slots is 0.53. We apply shear both parallel and perpendicular to the slots. The slip length is strongly dependent on the flow direction [38]. For parallel flow the slip length is positive, but for the perpendicular case it becomes negative. Flow direction affects also greatly on the shear-rate dependence (cf. Fig. 6, right). When flow is parallel to the grooves no shear-rate dependence is observed, but for the perpendicular case this dependence is similar to that seen on hole arrays. These results can be understood on the basis of deforming bubbles. For perpendicular flow the bubbles are able to deform, but for the parallel case the bubbles retain their shape regardless of the shear rate.
5 CONCLUSION

In this paper we present our applications of the lattice Boltzmann method to microfluidic problems. The focus of our research is laid on the validation of the no-slip boundary condition. By introducing a model for hydrophobic fluid-surface interactions and studying pressure-driven flow in microchannels, we show that an experimentally detected slip can have its origin in hydrophobic interactions, but is constant with varied shear rates and decreases with increasing pressure. Another effect that was not fully understood so far is the influence of surfaces roughness. We are able to apply our simulations to surface data obtained from AFM measurements of experimental samples. We show that ignoring roughness can lead to large errors in a detected slip. In fact, we propose that roughness alone could often be the reason for apparent boundary slip.

Microscale bubbles at surfaces allow to tailor the slip properties of a surface. Such a surface with bubbles may yield negative slip, i.e., increased resistance to flow, if bubbles are strongly protruding to the channel. Our simulations capture the deformability of bubbles and thus allow to study the influence of the shear rate on the deformation of the interface and its effect on the measured slip. We find that the slip decreases with increasing shear rate demonstrating that shear induced bubble deformation cannot explain recent experimental findings where slip increases with increasing shear rate [19].

In the current review, we also demonstrate the suitability of the lattice Boltzmann method for modeling microfluidic applications: in contrast to molecular dynamics, it is able to reach experimentally available time and length scales. This allows us to compare our results to experimental data directly and to simulate flow along surface data obtained from AFM measurements of “real” samples. Additionally, multiphase lattice Boltzmann simulations inherently contain the possibility to study dynamical experiments.

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References


Fig. 6  The left figure shows a snapshot of a bubble deformed by shear flow. In the centre, the slip length as a function of the capillary number for a square array of bubbles with three different protrusion angles, $\varphi = 63^\circ, 68^\circ$, and $71^\circ$ (from uppermost to lowermost) is shown. The inset shows cross sections of liquid-gas interfaces for four capillary numbers [38]. The right figure shows the slip length as a function of capillary number for a surface with cylindrical bubbles. Circles denotes the values for flow parallel to the bubbles and diamonds for the perpendicular direction.