Effects of Wall Boundary Conditions on Slip in a Nano-Channel 
Fluid Flow

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Term Project Report
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1 Motivation

In recent years, a large number of fluid devices have been fabricated which operate at the micro- and 
nano-scale. These devices have wide variety of applications [1], ranging from microfluidic actuators, 
microscale combustors, to on-chip heat pipes. While some of these devices exist only in a laboratory 
setting, some important small scale flow devices appear in common consumer products. For instance, 
the operation of modern hard disks heavily depend on the nano-scale gas flow between the hard disk 
head and the platter.

As these devices approach smaller and smaller scales, they begin to experience more and more phe-
nomena that lie outside the continuum regime. When the characteristic scale of the device \( H \) becomes 
comparable to the mean free path \( \lambda \) of the gas operating in the device, issues such as slip between the 
gas and solid interfaces arise. Fluid slip at the walls of these devices is of particular concern because it 
affects the shear stress seen by the walls, and the volume flow rate of the gas through the device, which 
are crucial parameters for their operation. At these small scales, the smoothness of the surface at the 
atomic level will also affect the flow, and must be taken into consideration.

2 Problem Statement

In this project, we examine the degree of fluid-wall slip in a three dimensional channel under varying 
temperature and wall roughness conditions using molecular dynamics (MD) simulations. Two configu-
rations of channel flow are considered: a shear-driven Couette flow and a pressure-driven Poiseuille flow 
(figure 1). In the continuum regime, the motion of the upper wall induces a linear velocity profile

\[
U(y) = U_w \frac{y}{H},
\]

while for Poiseuille flow the pressure gradient \( \frac{dP}{dx} \) causes a parabolic profile

\[
U(y) = -\frac{1}{2\mu} \frac{dP}{dx} (H - y) y,
\]
Figure 1: Schematic of (a) Couette and (b) Poiseuille flow in the continuum picture

for a given channel height $H$ and viscosity $\mu$. We define a slip length $l_s$ as

$$l_s = \frac{U(y = y_{\text{wall}})}{\left. \frac{dU}{dy} \right|_{y=y_{\text{wall}}}},$$

which characterizes the amount of slip at the wall at $y_{\text{wall}}$. For the no-slip boundary condition to hold, the slip length $l_s$ should be zero at the wall.

In this project we will determine the effect of temperature and wall boundary conditions, namely wall roughness, on slip length $l_s$.

3 Implementation

For the MD simulations we considered three-dimensional channels of wall-to-wall distance $H=6.33\,\text{a}_{\text{u}}$, length $L = 29.9167\,\text{a}_{\text{u}}$, and width $W=0.75\,\text{a}_{\text{u}}$, with a lattice constant of $a=5.31$ angstroms. To model the gas inside the channel, we used 2000 argon atoms interacting via a truncated Lennard-Jones 6-12 potential, with parameters $m=39.948$ a.u., $\sigma=3.405$ angstroms and $\epsilon_0 = 1.0325 \times 10^{-2}$ eV. The walls of the channels were formed by layers of solid argon atoms in a perfect (001) lattice configuration. For Couette flow, the atoms of the lower wall were fixed in space, while the atoms at the upper wall moved with constant velocity $U_w$ in the positive x direction. For Poiseuille flow, the atoms of the walls were fixed in space. However, the gas atoms were allowed to interact with the wall atoms through the same Lennard-Jones 6-12 potential with a higher energy constant $\epsilon_w = 10\epsilon_0$.

In the smooth wall channels, a single layer of an argon crystal lattice was sufficient at the top and bottom boundaries. In the rough wall case, we used two layers of lattice atoms, with every other unit cell of argon atoms removed from the inner lattice layer (see figure 2). Overall, creating the walls required 1440 atoms in the smooth wall case, and 2160 atoms in the rough wall case.

The code for these simulations was based on the MD++ code [6] from Prof. Cai, with some modifications to set up the channel geometry and to allow for separate wall and gas atoms. Additionally, we implemented the RPM membrane [5] discussed below and various boundary conditions specific to our problem.
3.1 RPM Membrane

To initiate a pressure gradient in Poiseuille flow, we used a reflecting particle method (RPM) membrane, as introduced by Li, Liao and Yip [5]. Following their method, we establish a fictitious membrane located at position $x = x_m$ in the channel, where particles traveling in the positive $x$ direction are allowed to pass freely. However, particles travelling in the negative $x$ direction may be reflected from the membrane with probability $P$, and may pass through the membrane with probability $1-P$ (see figure 3). Selectively bouncing particles allows this membrane to support a pressure difference on either side of $x_m$, and a negative pressure gradient $dP/dx$ across the length of the channel.

This method has the advantage of preserving the kinetic energy of particles which are reflected, and does not require rescaling of the kinetic energy to maintain the temperature of the system. Other methods, such as applying a body force to accelerate particles downstream, would inject energy into the system and require some means of dissipation for the channel flow to reach steady state.

In all Poiseuille cases, we located the membrane at $x=0.9L$ and gave it a finite thickness of 0.04L. The relevant statistics were gathered away from the membrane (see section 3.4). In order to have the membrane quickly establish a pressure gradient throughout the channel, we set $P=1.0$.

3.2 Boundary and initial conditions

We imposed periodic boundary conditions in all three directions of the simulation cell. In the Poiseuille simulations both upper and lower wall atoms are fixed, but in the Couette case the upper wall is set to move at a uniform velocity of $U_w = 0.01 a/dt$, and the lower wall is fixed.

While all of the wall atoms are positioned according to the fcc lattice structure, the gas atoms are initially randomly dispersed throughout the channel. The gas atoms also have no initial mean velocity.
at the start of the simulation, but are given a random thermal fluctuation according to the desired temperature \( T_0 \). To simulate the effect of having walls also at a temperature \( T_0 \), atoms that pierce the walls to cross the \( y \) boundaries of the simulation cell are re-initialized with a velocity fluctuation also at \( T_0 \). Most of the velocity re-initializations occurred during the equilibration process of the simulation, when frequent collisions between gas atoms produced high-velocity particles that very quickly reached the \( y \)-boundaries of the simulation cell.

### 3.3 Simulations

A number of Couette and Poiseuille flow simulations were carried out in the temperature range 300-500K and with the two different wall models. The different cases simulated are listed in table 1.

For the Couette flows, we equilibrated the channel flow over a period of 30,000 timesteps for a total of 0.225 ps. The simulation was then run for an additional 80,000 timesteps, or 1.6 ps to gather the necessary statistics. For the Poiseuille flows, we equilibrated the system for 1.0225 ps using 70,000 timesteps total, and then run for another 3.2 ps, or 80,000 timesteps to gather data. To monitor the progress of the channel flow equilibration, we examined the mean velocity \( U \), averaged over all directions, in the channel at every 100 timesteps. Starting from a zero mean velocity, the Couette flow configuration required about 15,000 steps to achieve a mean velocity of about \( 3 \times 10^{-3} \) \( a / \Delta t \) (see figure 4).

These simulations were carried out on Pentium III and Pentium 4 Linux PCs. Each simulation took about 3 to 5 hours to reach equilibrium, and then another 10-12 hours to run. Time steps of about 0.02-0.04 fs were used for the simulations.

### 3.4 Post-processing

The simulations provided raw data in terms of particle positions and velocities in the channel. A set of MATLAB routines were written to process this raw data.

For the Couette flow simulations, data from the entire length of the channel was used to compute average statistics. For the Poiseuille flow simulations, the presence of the RPM membrane creates an
Figure 4: Couette flow equilibration. The average velocity $U$ of all particles is initially 0 at step 0, and settles to an equilibrium after about 15,000 steps.

<table>
<thead>
<tr>
<th>No.</th>
<th>Simulation</th>
<th>Lower Wall</th>
<th>Upper Wall</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Couette</td>
<td>Smooth</td>
<td>Smooth</td>
<td>300</td>
</tr>
<tr>
<td>2</td>
<td>Couette</td>
<td>Smooth</td>
<td>Smooth</td>
<td>400</td>
</tr>
<tr>
<td>3</td>
<td>Couette</td>
<td>Smooth</td>
<td>Smooth</td>
<td>500</td>
</tr>
<tr>
<td>4</td>
<td>Couette</td>
<td>Rough</td>
<td>Rough</td>
<td>300</td>
</tr>
<tr>
<td>5</td>
<td>Couette</td>
<td>Rough</td>
<td>Rough</td>
<td>400</td>
</tr>
<tr>
<td>6</td>
<td>Couette</td>
<td>Rough</td>
<td>Rough</td>
<td>500</td>
</tr>
<tr>
<td>7</td>
<td>Poiseuille</td>
<td>Smooth</td>
<td>Smooth</td>
<td>300</td>
</tr>
<tr>
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<td>Poiseuille</td>
<td>Smooth</td>
<td>Smooth</td>
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<td>13</td>
<td>Poiseuille</td>
<td>Smooth</td>
<td>Rough</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 1: List of simulations carried out
artificial gradient in density across the membrane, with low particle density to the left of the membrane and high particle density to the right of the membrane. A snapshot (Figure 5) of the atom positions from simulation No. 13 clearly shows this effect of the RPM membrane. Hence the data near the membrane (which is located at $x_m = 0.9 * L$) has to be ignored. The region between $x = 0.2 * L - 0.6 * L$ was used to compute the average statistics for the Poiseuille flow simulations.

Since the average velocity profiles of both Couette and Poiseuille flow depend only on $y$, the velocities were averaged out in the $x$ and $z$ directions. A moving bin average was used to compute the $y$ variation of velocity. At any given point $y$, the velocity of all the particles falling inside a bin of size $0.1 * H_t$ centered around $y$ was averaged out to obtain the velocity of the fluid at $y$. A discussion of the results obtained is presented in the next section.

4 Discussion of Results

4.1 Averaged velocity

Except for slip at the boundaries, the averaged velocity profiles obtained from the Couette and Poiseuille flow simulations agree with the theoretical results for continuum fluid flow. The Couette velocity profile is linear across the height of the channel, while the Poiseuille velocity profile is parabolic. However, as we had expected, we do observe some slip at the walls.

In the smooth wall Couette simulations (#1, 2, 3), increasing the temperature from $T=300$ K to $T=500$ K had little effect on the averaged velocity profile (see figure 6(a)). In these plots, the distance $y$ has been normalized by the total channel height $H_t$ (including the wall thickness), while velocity $U_{avg}$ had been normalized by the velocity of the upper wall $U_{wall}$. The rough Couette simulations (#4, 5, 6) is shown in figure 6(b), and for these cases, increasing temperature also did not affect the overall velocity profile to a significant degree.

The average velocity profiles for the Poiseuille flow simulations have been shown in figure 7. Here the velocity is normalised by $a/dt$, the lattice constant divided by the time step of the simulation. It is interesting to note that the average velocity profile in the rough wall Poiseuille flow does not appear to depend heavily on temperature from $T=300$K to $500$K, but in the smooth wall case, the velocity profile at $T=300$ K is significantly higher than at other temperatures.

As expected from continuum theory, the averaged V and W velocities (velocities in the y and z directions) are small when compared to the streamwise velocity. As shown in figure 8 for Couette
Figure 6: Averaged velocity profiles for Couette flow. In the smooth wall cases (a), the horizontal lines denote the location of the lower and upper walls in the simulation cell. In the rough wall cases (b), the double horizontal lines denote location of the top and bottom surfaces of the bumps on the wall.

Figure 7: Averaged velocity profiles for Poiseuille flow. In the smooth wall cases (a), the two gray lines denote the location of the lower and upper wall. In the rough wall cases (b), the gray lines denote the top and bottom surfaces of the bumps on the wall.
simulation #1, the maximum averaged $V$ velocity is about 2% of the wall velocity, while the maximum averaged $W$ velocity is about 5% of the wall velocity.

4.2 Slip length

Estimating slip length has been a difficult task with the bin averaging technique we have used for estimating the average velocity profile. An accurate estimation of average velocity and velocity slope at the walls is necessary to estimate slip length. Having very small bins made the velocity profile wavy, while giving very good spatial resolution. Using larger bins, while producing smoother average velocity profiles, reduced the spatial resolution and hence gave incorrect average velocity and slope at the wall. We had decided to go with small bin sizes of $0.02 \times H_t$, which appear to predict at least the velocity at the wall correctly. These estimates of slip hence must be taken with a “pinch of salt”, especially for the Poiseuille flow configurations. The slip length estimates for Couette flow configurations are more reliable, since we have an almost constant slope for the average velocity through most of the channel height. Li, Liao and Yip [5] provide a working, but very elaborate way of working around this problem, by smoothing the data using a polynomial interpolation technique.

For the Poiseuille configurations, slip lengths of around $0.15 \times H_t$ and $0.05 \times H_t$ were found for the bottom wall in both smooth and rough configurations, irrespective of the temperature. The slip lengths for the lower stationary wall in the Couette cases are plotted in figure 10. We again see a reduction in slip length from about $0.18 \times H_t$ to $0.02 \times H_t$ with wall roughness. For the rough walls in both flows, the velocity used to compute slip was measured at the middle of the rough portion of the wall lattice, that is at $\frac{1}{2}(y_b + y_h)$, where $y_b$ and $y_h$ correspond to the top and bottom of the wall bumps. We see that roughness has greatly helped in reducing slip. Figure 9 is a plot of the average velocity profile from
Poiseuille simulation No. 13. The lower wall is smooth while the upper one is rough. It is very clear from here that the roughness has reduced slip considerably.

We note that the slip doesn’t vary too much with temperature for the Couette cases. This could be expected, given that there is not much variation in the mean velocity profile with temperature (see figure 6). From continuum theory, the mean velocity for Couette flows is independent of the temperature of the gas.

5 Summary and Conclusions

The MD simulations of Couette and Poiseuille channel flow that we performed, while generally confirming the validity of the mean flow profiles from continuum theory away from the walls, show slip at the walls depending on the wall roughness. This slip has profound effect on flow rate and stresses at walls, given the small size of the channels in micro- and nano-scale devices. Hence it is important to be able to estimate the magnitude of slip.

From our simulations we found that wall roughness played a much greater role in determining slip than temperature. This is in agreement with some previous works [6], which found that surface roughness on the scale of the mean free path of the gas atoms helped to reduce the slip length in channels. However, the range of temperatures (from T=300K to 500K) explored in this project is fairly limited and would sample only a small range of Knudsen numbers. Future studies might extend the range of temperatures and density of the gas in the channel, and see if the same results hold.
Figure 10: Variation of slip length with temperature for the Couette simulation

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References


