# Worksheet 4: Flow Between Plates and Free Energy

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## Contents

## General Remarks

- Deadline for the report is **Monday, 19th of June 2017, 12:00 noon**

- In this worksheet, you can achieve a maximum of 20 points.

- The report should be written as though it would be read by a fellow student who attends the lecture, but doesn't do the tutorials.

- To hand in your report, send it to your tutor via email.

  - David (`david.sean@icp.uni-stuttgart.de`)

- Please attach the report to the email. For the report itself, please use the PDF format (we will *not* accept MS Word doc/docx files!). Include graphs and images into the report.

- The report should be 5–10 pages long. We recommend using LaTeX. A good template for a report is available online.

- The worksheets are to be solved in **groups of two or three** people.

# 1    Introduction

This tutorial is divided in two separate parts: i)Flow between plates and ii)Thermodynamic integration. For the first two questions, you will study the laminar flow profile of a fluid between two infinite plates. For the last question, you may want to read parts of the book:
Understanding Molecular Simulation (2nd Edition), From Algorithms to Applications by Frenkel and Smit, 2001. Academic Press, ISBN: 9780122673511
From an ICP CIP-pool computer, you can find the seventh chapter under:
/group/sm/2017/tutorial_04/Frenkel-Smit-Chap7.pdf
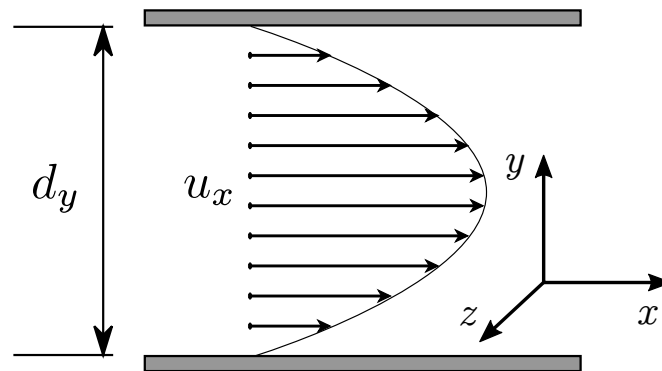
# 2    The flow between two infinite plates



**Figure 1:** The parallel plate geometry with the steady-state fluid velocity profile.

You need to characterize a microfluidic system that has microscopic length scales. The geometry under consideration consists of two fixed infinite parallel plates separated by a distance $d_y$ shown in Fig. 1. The fluid has no-slip boundary conditions next to the walls (it has zero velocity) given by

$$\boldsymbol{u}(x, y = 0, z) = 0$$
$$\boldsymbol{u}(x, y = d_y, z) = 0$$

There is a constant force density $\boldsymbol{f}$ oriented in the positive $x$-direction such that a steady-state fluid velocity profile similar to that show in Fig. 1 is established. Thinking ahead, this will be modelled in a periodic simulation box, thus there there is no pressure difference across the system, i.e., the flow is only created via the external force density $\boldsymbol{f}$.

## 2.1 Analytical solution

> **Task** (6 points)
>
> - Starting with the Navier Stokes equations shown in class (explicitly indicate all steps and assumptions.):
>
> $$\rho \left( \frac{\partial}{\partial t} \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right) = -\nabla p + \eta \nabla^2 \boldsymbol{u} + \boldsymbol{f},$$
>
> $$\nabla \cdot \boldsymbol{u} = 0,$$
>
> derive the shape of the steady-state velocity profile.
>
> - What is the maximum velocity? Where is it located?

**Hint**

- You can assume there the fluid flow is in the $x$-direction only (unidirectional).

- You can assume there the fluid velocity profile only changes in $y$ direction.

## 2.2 Computer simulations

The velocity profile can be obtained from computer simulations using the Lattice-Boltzmann method with ESPResSo. You will need to compile ESPResSo with either the GPU or CPU implementation. It is easiest to follow the installation steps from previous worksheets, but this time when editing `myconfig.hpp`, enable the three following features:

```
EXTERNAL_FORCES
LB_GPU
LB_BOUNDARIES_GPU
```

by removing the comment symbols '`//`'. If you are using a computer in the CIP pool, it is recommended to use the faster GPU implementation. You may use uncomment the features `LB` and `LB_BOUNDARIES` instead to use the CPU implementation.

You will compare the numerical results with the analytical solution. The simulations will take place in a periodic cubic simulation box of size $32 \times 32 \times 32$. The walls are modelled using an LB boundary which are placed at an offset of 1.5 between the top and bottom limits resulting in $d_y = 28$ (between $y = 1.5$ and $y = 29.5$). You will need to adapt the analytical solution by adjusting to these boundary conditions.

**Equilibration Time**

Now we can start with the real simulations. Take a look at and make sure to understand the template python script from the course webpage.

**The velocity profile**

Finally, the complete velocity profile can be measured. Make sure the system is equilibrated (steady state is reached) and plot the velocity profile between the plates (at $y = 1, 2...31, 32$).

**Hint**

- Make sure to adjust the analytical solution with the boundary conditions from the simulations.

# 3 Free Energy calculations

This question is taken from chapter seven from Frenkel and Smit, which covers computational techniques to investigate the free energy. An alternative method for calculating the free energy difference between state $A$ and state $B$ is to use an expression involving the difference of the two Hamiltonians:

$$F_A - F_B = \frac{-\ln\left[\langle \exp\left[-\beta\left(\mathcal{H}_A - \mathcal{H}_B\right)\right]\rangle_{N,V,T,B}\right]}{\beta}$$

**Hint**

- To derive the equation, start with Eq (7.1.1) of Frenkel and Smit.