Study of Poiseuille flow in a slit pore

Carlos Braga and Jordan Muscatello

Department of Chemical Engineering, Imperial College London, SW72AZ UK

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1 Introduction

Classical Navier-Stokes (NS) hydrodynamics is known to describe macroscopic flows of simple fluids. In systems where the state variables such as temperature and density vary markedly over a scale comparable to the molecular mean free path, these equations start to break down [1, 2]. In particular, the non uniform nature of an interfacial fluid makes the microscopic representation of mass, momentum and energy fluxes significantly more complex to compute [3, 4] causing in this way the failure of microscopic defition of local transport coefficients in a confined medium using bulk approximations.

1.1 Navier-Stokes hydrodynamics for gravity flow

In this exercise we will consider a gravity driven flow in the x direction between two closely spaced parallel plates. The normals of these surfaces are perpendicular to the direction of the gravity force, i.e., in the y direction. Fig. (1) illustrates a snapshot of the system. The wall atoms are depicted in grey and the fluid atoms in blue respectively. The NS equation of motion for the fluid in this system is given by

$$\rho \frac{\mathrm{d}\,\mathbf{u}}{\mathrm{d}\,t} = -\nabla \cdot \mathbf{P} + n\,\mathbf{F}_e \tag{1}$$

where $\mathbf{F}_e$ is the magnitude of the external field is defined here simply by the molecular mass of the fluid particles, m, multiplied by the gravity acceleration g. The number and mass densities are given by n and ρ respectively, and $\mathbf{u}$ is the fluid streaming velocity. The pressure tensor in given by $\mathbf{P}$. If the fluid is isotropic, the we can decompose the pressure tensor into a viscous and an hydrostatic component $\mathbf{P} = \mathbf{\Pi} + p\mathbf{I}$, where $\mathbf{\Pi}$ is the viscous pressure tensor, $\mathbf{I}$ is the isotropic second rank tensor and p is the scalar hydrostatic pressure.

In the particular case of a gravity driven flow, the steady state equation of motion is given by

$$\frac{\mathrm{d}\,\Pi_{yx}}{\mathrm{d}\,y} = n\,F_e \tag{2}$$

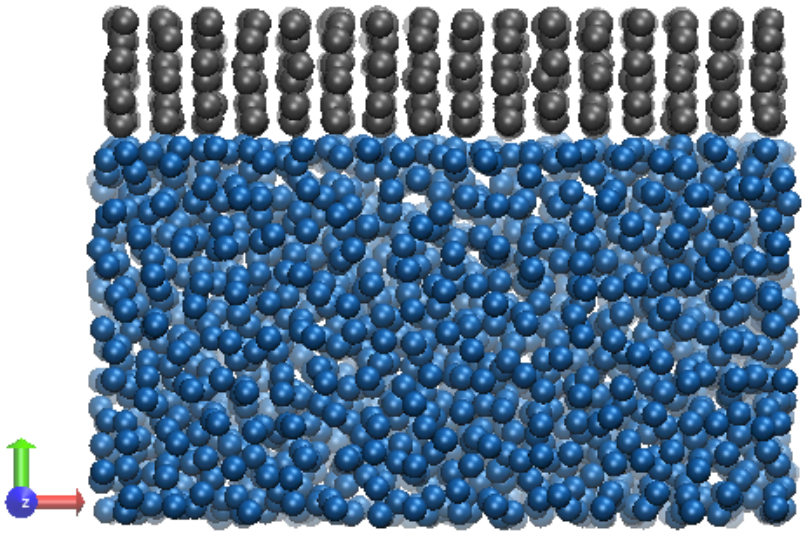

Figure 1: Snapshot of a fluid undergoing planar Poiseuille flow. The z axis is normal to the page. Because we are applying periodic boundary conditions, there is only one single plate. The fluid below will interact with the wall above.

where Π_{yx} is defined here as the flux of momentum in the x direction by molecular interactions on a surface normal to the y direction. When there are no spatial variations in the fluid density, the shear stress profile will be linear. In reality, the presence of the pore walls and the nonuniform character of the temperature profile results in variations of the density across the pore channel, yielding a non-linear stress profile. For a Newtonian fluid, the shear viscosity is assumed to be constant and the shear stress is given by

$$\Pi_{yx} = -\eta \frac{\mathrm{d}\, u_x\,(y)}{\mathrm{d}\, y} \tag{3}$$

Combining Eq. (2) and Eq. (3) with the assumption that the flow velocity takes the form $\mathbf{u} = [u_x\,(y)\,, 0, 0]$ we have

$$\eta \frac{\mathrm{d}^{\,2}\, u_x\,(y)}{\mathrm{d}\, y^2} = -n\, F_e \tag{4}$$

Solving Eq. (4) for the flow velocity with stick boundary conditions ($u_x\,(\pm\, W/2) = 0$) gives the classical quadratic profile for Poiseuille flow

$$u_x\,(y) = \frac{n\, F_e\, W^2}{8} \left[1 - \left(\frac{2\, y}{W}\right)^2\right] \tag{5}$$

where W is the fluid channel width. This expression is expected to break down for channels which have a width of only a few molecular diameters wide. The objective of

this exercise is to test the validity of Eq. (5) by performing a set of NEMD simulations of Poiseuille flow of a Lennard-Jones fluid.

1.2 Simulation details

The NEMD techniques used to simulate planar Poiseuille flow can be found in the work of Travis *et al.* [2, 5] and Todd *et al.* [6, 7]. Here we only briefly outline the way in which the simulations are carried out. For a fluid system confined between two parallel walls, *cf.* Fig. (1), a constant force in the x direction is applied to each fluid particle. The geometry of the system is described by Fig. (2). Both the fluid and the wall particle interact through a purely repulsive WCA interatomic potential

$$\phi(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] + \epsilon_{ij} \quad r < r_{cut} \tag{6}$$

where r is the scalar distance between a pair of interacting atoms of components i and j respectively. The corresponding energy and length scales are defined by ϵ_{ij} and σ_{ij} respectively. Unless otherwise indicated, reduced units are used throughout this work, i.e., $\sigma_{ii} = 1.0$ and $\epsilon_{ii} = 1.0$. The cutoff radius is given in reduced units by $r_{cut} = 2^{1/6}$ which is the distance of the Lennard-Jones potential minima.

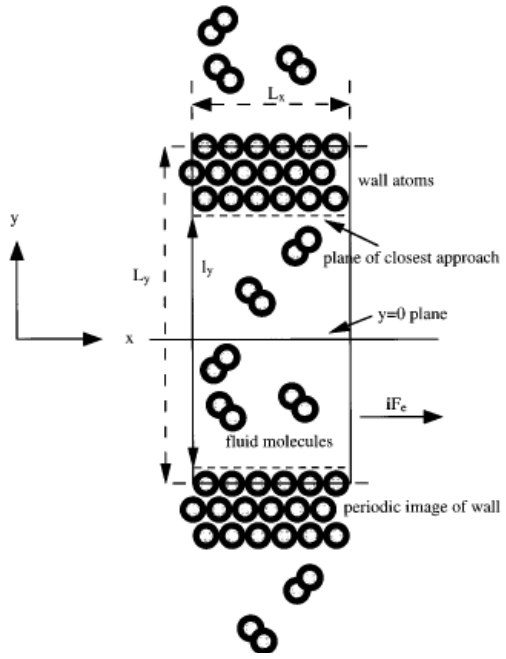

Figure 2: Simulation geometry for planar Poiseuille flow. The z axis is normal to the page

In this exercise we examine two channel widths, $W = 5.1$ and $W = 10.2$. Here W is defined as the separation in the y direction between the centres of the first layer of wall

atoms adjacent to the fluid. Both systems consisted of the same number of wall particles $N_w = 768$ arranged in a fcc lattice of cell dimensions $\{8, 3, 8\}$ resulting in a wall three atomic layers thick (256 atoms per layer) in the y direction. The number of fluid atoms is $N_f = 1000$ for the smaller channel width $W = 5.1$ and $N_f = 2000$ for $W = 10.2$.

The wall atoms are tethered to their corresponding lattice points through a set of harmonic restraining forces with a spring constant $k_s = 150.15$. The wall dimensions are given by $L_x = L_z = 16.6$ and $L_w = 2.2$ resulting in a wall density of $n_w = 1.27$ and a fluid geometric density of $n_f = 0.711$. The walls on both systems are kept at a constant temperature $T = 0.722$ using a Nosé-Hoover thermostat [8] with the centre of mass velocity removed from the velocities of each wall.

2 Getting the files

Before starting this exercise, you will need to obtain the necessary files. Login to your account on the Imperial cx1 cluster, and then run the command

```
$ git clone https://github.com/niallj/ImperialNESS-Sep14.git
```

This will create a folder called ImperialNESS-Sep14 in your home folder that contains the files that you will need for all of the exercises.

3 Running the simulations

All simulations will be performed using the LAMMPS simulation package [9]. The exercise folder contains two directories named `poreW_5_1` and `poreW_10_2` containing the simulations files corresponding to each pore dimension. Each directory will contain two subfolders `simulation` and `analysis`. The `simulation` subfolder contains four LAMMPS input files and bash scripts to submit to the cluster PBS job resource manager. More information about the Imperial College HPC queuing system can be found here. All of the files contain comments explaining what each of the commands does. The `analysis` subfolder contains a set of scripts to analyse the computed profiles using the gnuplot package and to visualise the trajectories using VMD [10].

1. Read through the files to make sure you understand what is taking place. **Please ask if you have questions!**

2. Submit the equilibration jobs. These should not take long to complete.

3. Plot the data in the `0.out.sample` file to see if your system has reached equilibrium. If it has, you can use the restart files that you have generated to run a production simulation. If not, adjust the parameters in your input file and try again.

4. Submit the production jobs. These will take a bit longer to complete. While you wait, you can visualise the trajectories or start the next section. Besides the two subfolders mentioned above, there is an additional subfolder named `results`. It

contains the results from a previous long production run. If the simulations take too long, you can run a shorter simulation and compare your results with the previous ones.

4 Analysing the simulations

Hopefully, the simulations you submitted will now be finished. Use the supplied code to perform the analysis. The analysis procedure is equivalent to both pore systems. For each one plot property profiles.

1. How does the density profile change with pore dimensions?
2. What is the shape of the profiles for the velocity in each Cartesian direction?
3. Plot the shear stress profile and try to understand the meaning of its value.
4. Because the walls are thermostated, there will be a heat flow from the viscous heating of the fluid towards the walls. Plot the heat flux profile and interpret its meaning.

5 Experiment with systems

1. The WCA potential means that all atomic interactions are purely repulsive. What would be the effect of including the attractive part of the potential in the inter atomic interactions. Try to change the cutoff radius to $r_{cut} = 2.5$ and repeat the analysis. Compare with the reference results.
2. A different way of controlling the system temperature is to apply a thermostat to the fluid particles. Because the fluid is flowing, the kinetic energy of each atom in the fluid will have two contributions, a thermal one and a convective one resulting from the application of the external force. To properly thermostat the fluid, one needs to remove a spatially averaged centre of mass velocity field before computing the energy. Try to change the thermostat method using a profile-unbiased thermostat [11].
3. Higher field strengths will result in a higher fluid streaming velocity and a higher viscous dissipation rate. How does this affect the temperature profile of the fluid? Try to increase the value of the external field and compare.

References

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