Project2 - FYS4460

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f) Diusion in a nano-porous material

I have followed the description from question a-e. The lennard fluid is first thermalized at $T = 0.851$ with a density corresponding to the unit cell length of 5.72 Å with fcc packing. We we measure the mean square displacement (msd) in the nano-porous material. The result is shown in figure 1.

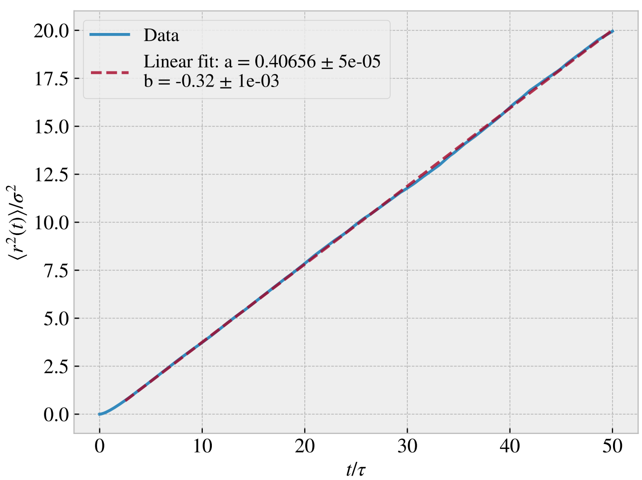

FIG. 1. Mean square displacement $\langle r^2(t)\rangle$ as a function of time.

We estimate the diffusion constant from the relaiton

$$\langle r^2(t)\rangle = 6Dt, \quad when\ t \to \infty \tag{1}$$

From the linear fit on figure 1 we estimate the diffusion constant as

$$D_{\text{nano-porus}} = 6.776 \times 10^{-2} \pm 8 \times 10^{-6}$$

g) Flow in a nano porous material

Darcy's law is given as

$$U = \frac{k}{\mu}(\nabla P - \rho g)$$

Where U is the volume flux (volume per area and time), k is the permeability of the medium, μ is the viscosity, ∇P is the pressure drop over a given distance, ρ is the density and g is the gravitational acceleration.

We can relate the gravitional force as $F_G = mg$, thus we can rewrite the term ρg as

$$\rho g = nmg = nF_G$$

We can assume that gravity acts in x-direction such that $F_G = F_x$ and we get

$$U = \frac{k}{\mu}(\nabla P - nF_x)$$

h) Measure flow profile in pipe

We use the same system consisting of $20 \times 20 \times 20$ unit boxes and carve out a cylinder along the x-axis with radius 12 Å. Everything outisde the cylinder is frozen while the atoms inside can move freely. The freely moving atoms is reduced to half density. We add a force $F_x = 0.1\ \epsilon/\sigma$ on every free atom in the x-direction. We then let the system stabilize and measure the flow profile, that is the velocity in x-direction as a function of radial distace to the x-axis.

We run the simulations for almost 450 τ (the simulation suddently crashed at this point). We calculate the innerproduct for the velocity distribution as

$$\frac{\sum_i h_i(t)h_i(t_n)}{\sum_i h_i(t_n)^2} \tag{2}$$

where h_i is the height of radial bin i in the histogram and t_n is the final time-step. We then plot this to confirm that the cistirbution is converging towards a steady state (see figure 2).

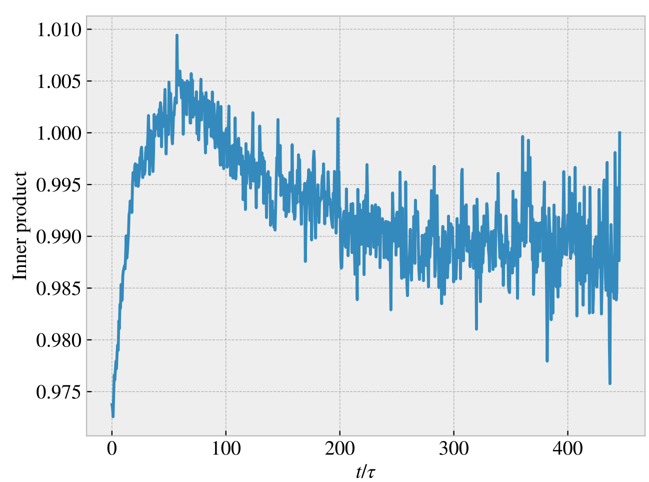

FIG. 2. The inner product (equation 2) for the velocity distribution $v_x(r)$ with radial bins. We see that the distirbution is somewhat reaching a steady state towards the end. We also notice bigger fluctuations which can probably be connected to the crash of the simmulaitons at the end.

Theoretically we expect the flow profile to follow:

$$u(r) = \frac{G}{4\mu}(R^2 - r^2)$$

(equation 4.27 in [1]), where R is the radius of the cylinder and $G = |\Delta P|/L$ with

$$\Delta P = p_1 - p_2 = \rho g(h_1 - h_2) - \rho g L$$

(equation 6.2 in [1]). Since we have no height difference in this system we only have a contribution from the hydrostatic pressure $\rho g L$. In addition we swapped the gravity with the force F_x and we get

$$G = |-\frac{nF_x L}{L}| = nF_x$$

From this we expect the flow profile in x-direction to follow the relation:

$$v_x(r) = \frac{nF_x}{4\mu}(R^2 - r^2) \quad (3)$$

By making a linear fit between $y = v_x(r)$ and $x = (R^2 - r^2)$ we can estimate the value $\frac{nF_x}{4\mu}$ as the slope on the fit a as shown in figure **??**

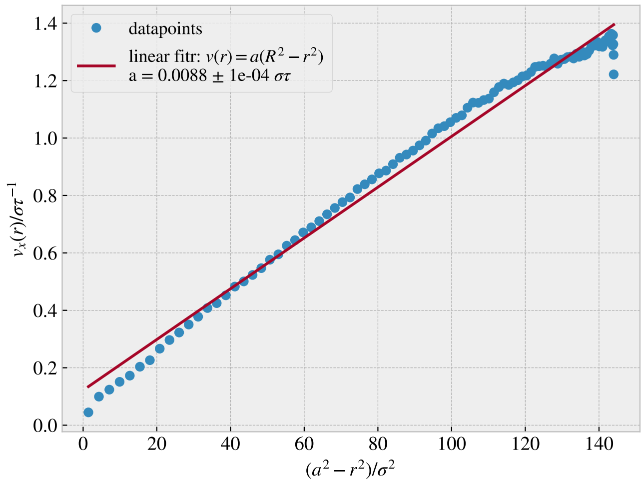

FIG. 3. Linear fit from relation 3.

The actual profile is shown along side with the fit in figure 4

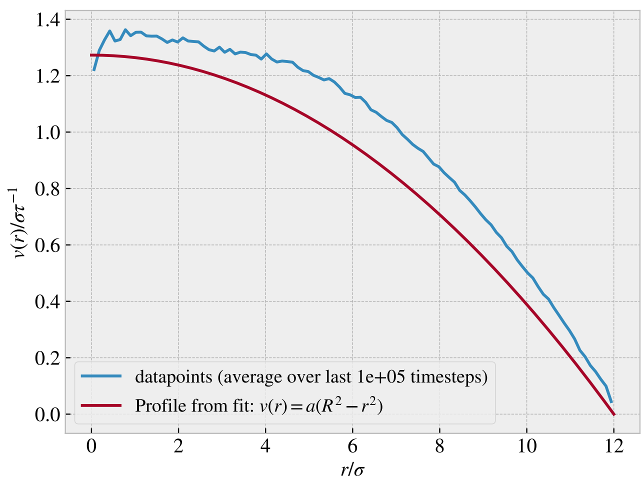

FIG. 4. Expermental and fitted velocity profile.

From the fit shown in figure 3 we estimate the viscosity μ to be

$$\mu = \frac{nF_x}{4a} = 1.19 \pm 0.01$$

[1] Jens Feder, Flow in Porous Media