FYS4460: Project 2
Advanced Molecular Dynamics Modeling

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Abstract

The molecular dynamics of a nano-porous material consisting of Argon atoms is modeled by developing a computer program. Using a Lennard-Jones potential the diffusion in, flow through, and deformation of a nano-porous matrix are measured and characterized.

Keywords: Molecular dynamics, Argon, Lennard-Jones potential, Nano-porous material, Cylindrical pores, Spherical pores, Diffusion constant, Spatial distribution of the pressure, Porosity, Flow profile, Viscosity, Permeability

Cylindrical pore

In this exercise we cut out a cylindrical pore of radius $2nm$ at the center of the system. In Fig. 1 and Fig. 2 we have visualized a $16 \times 16 \times 16$ and a $20 \times 20 \times 20$ Argon system, respectively. From these figures we see the cylindrical pore at the center of the system and the matrix, which consists of non-moving atoms, surrounding the pores.

Spherical pores

In this exercise we generate a matrix consisting of 20 pores at random positions and with random radius uniformly distributed between $R_0 = 2nm$ and $R_1 = 3nm$. The porosity of the generated system is measured to be $\phi = 0.43$. The porosity is defined as the relative amount of pore space in the

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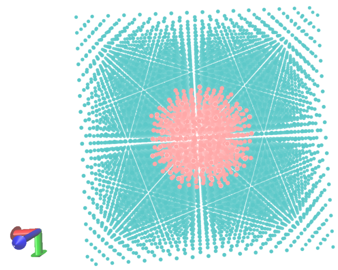
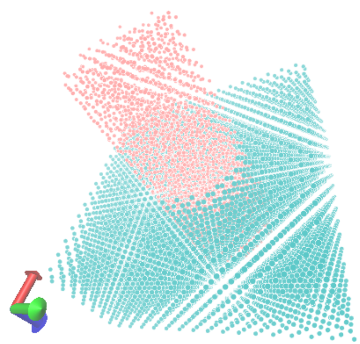


(a)



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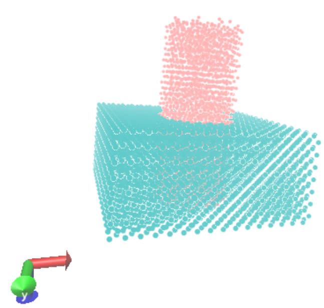
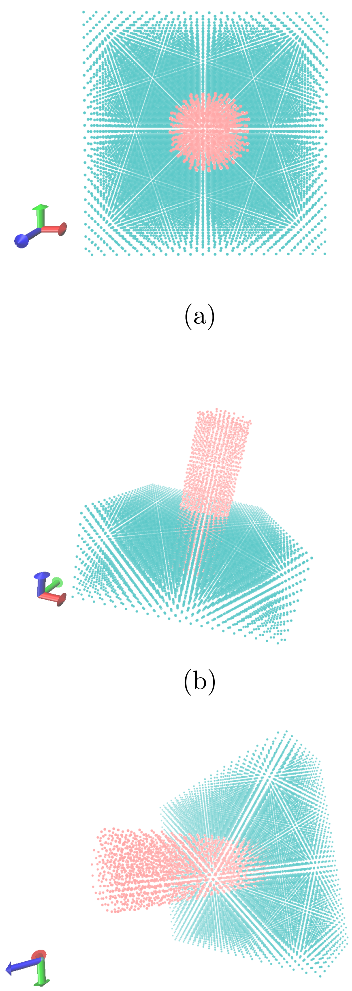


(c)

Figure 1: Visualization of $16 \times 16 \times 16$ Argon atoms.



(a)

(b)

(c)

Figure 2: Visualization of $20 \times 20 \times 20$ Argon atoms.

volume. The total volume of the matrix is given by

$$V_{Matrix} = \sum_{i=1}^{20} V_i = \sum_{i=1}^{20} \frac{4}{3}\pi R_i^3 = \frac{4}{3}\pi \sum_{i=1}^{20} R_i^3.$$

The porosity takes then the following form

$$\begin{aligned}\phi =& \frac{V_{Pore}}{V} \\ =& \frac{V - V_{Matrix}}{V} \\ =& \frac{L^3 - \frac{4}{3}\pi \sum_{i=1}^{20} R_i^3}{L^3} \\ =& 1 - \frac{4}{3}\frac{\pi}{L^3}\sum_{i=1}^{20} R_i^3. \end{aligned} \tag{1}$$

Temperature evolution of the porous medium

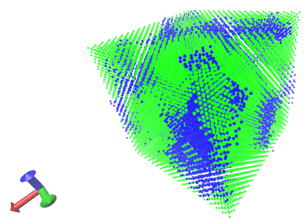
In figure 4 we have plotted the time evolution of the temperature for the porous medium consisting of $20 \times 20 \times 20$ Argon atoms. The matrix consists of 20 spheres randomly placed in the system and with random radius.

The spatial distribution of the pressure

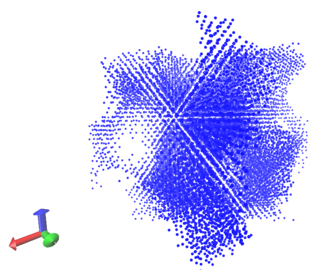
In order to measure the spatial distribution of the pressure, we have divided the hole system into equally sized cells, and we have calculated the pressure inside each cell. The result is visualized in Figs. 5 and 6. From these figures we see that the pressure is equal to zero at places where we have our matrix, which is what we would expect. Inside the pores, where we have freely moving Argon atoms, we see a non-zero pressure.

Diffusion in a nano-porous material.

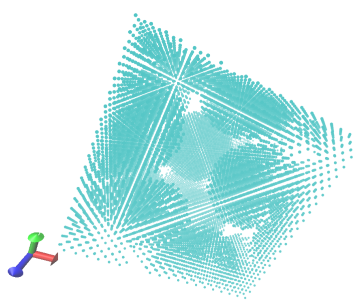
In this exercise we have measured the mean square displacement, $\langle r^2(t) \rangle$, at $T = 1.5$ and for the low-density fluid. The result is visualized in Fig. 7. From this figure we see that the mean square displacement is linearly increasing. Based on linear fitting we found the following numerical value for the diffusion constant: $D_{179.61K} = 5.54 \times 10^{-4}$.



(a) Porous sytem



(b) The pores



(c) The matrix.

Figure 3: Visualization of porous system consisting of $20 \times 20 \times 20$ Argon atoms. The matrix consists of 20 spheres randomly placed in the system.

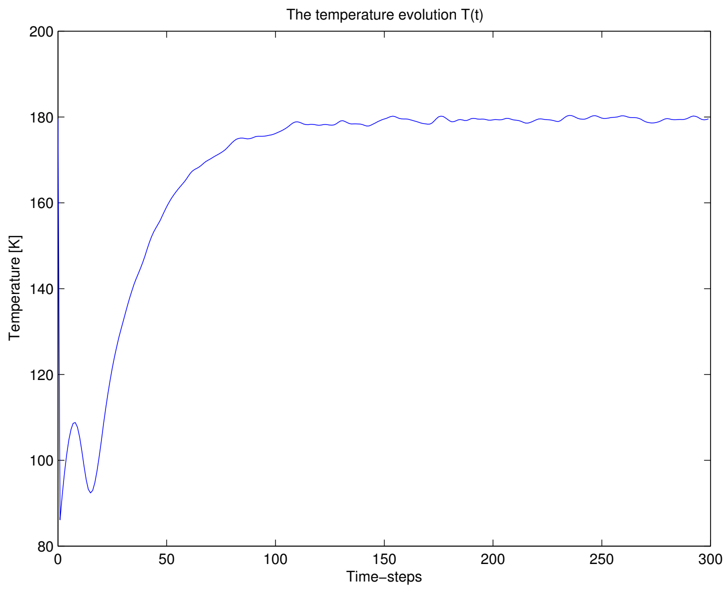


Figure 4: The temperature evolution of the porous medium consisting of $20 \times 20 \times 20$ Argon atoms.

Flow in a nano-porous material

We can induce flow in the material by introducing an external force, $\vec{F} = F_z\hat{i}$, acting on each atom. In the case of flow in a gravitational field, Darcy's law is usually formulated as:

$$U = \frac{k}{\mu}\left(\nabla P - \rho g\right). \tag{2}$$

We know that the mass density is defined as

$$\rho = \frac{M}{V} = \frac{Nm}{V}, \tag{3}$$

where m is the mass of each particle, N is the total number of particles and V is the total volume of the system. We also know that the number density of atoms is defined as $n =: N/V$, therefore we can write Eq. (3) as

$$\rho = nm. \tag{4}$$

From Newton's second law we have

$$F = ma = mg. \tag{5}$$

Substituting m from Eq. (4) into Eq. (5), we obtain

$$F = \frac{\rho}{n} g, \tag{6}$$

which can be rewritten as

$$nF = \rho g. \tag{7}$$

Therefore, we have shown that we can replace ρg by nF_z in Eq. (2).

We know that for a cylindrical pore the flow profile is given by

$$u(r) = \frac{\Delta P}{L} \frac{1}{4\mu} (a^2 - r^2). \tag{8}$$

Since all particles were subject to the force $F_z = 0.1\epsilon/\sigma$, we can rewrite the above equation as

$$\begin{aligned} u(r) &= \frac{NF_z}{V} \frac{1}{4\mu} (a^2 - r^2) \\ &= \frac{nF_z}{4\mu} (a^2 - r^2). \end{aligned} \tag{9}$$

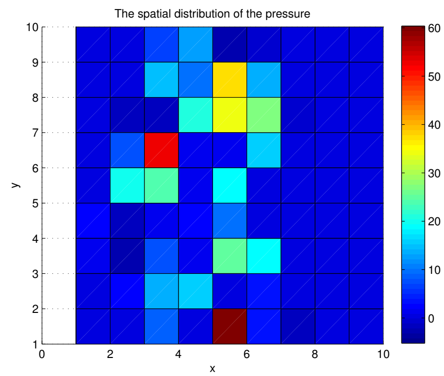
In Fig. 8 we have plotted the flow profile for a $8 \times 8 \times 8$ Argon system. From this figure we see that the flow profile has the expected form. The z-component of the velocity is highest at the center of the pore, and as we move away from the center the velocity tends zero, and it is equal to zero at the boundaries and outside the pore. By using equation (9), we have measured the viscosity in our system, and we have found $\mu \approx 8 \times 10^{-3}$.

Permeability

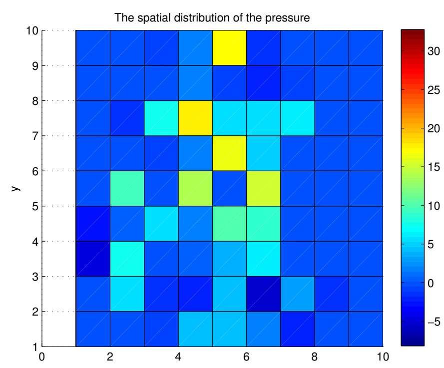
We know that the permeability for a cylindrical pore is proportional to the probity of the system

$$k = \frac{\phi a^2}{8}, \tag{10}$$

where a is the radius of the cylinder. For our system we have $\phi = 0.213$ and $a = 1.5nm$. With this values we find that the permeability is equal to $k \approx 6$ Å^2.

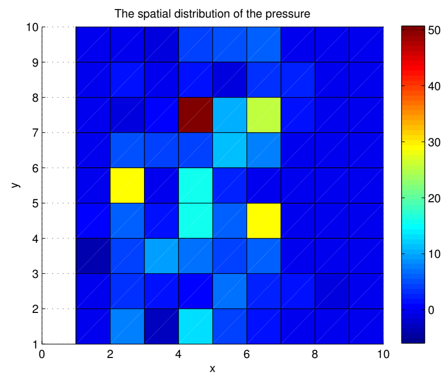


(a) The spatial distribution of the pressure at $t = 10$

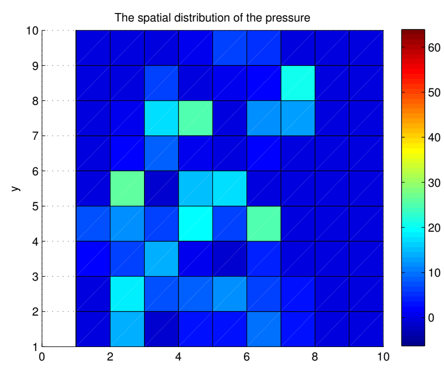


(b) The spatial distribution of the pressure at $t = 20$

Figure 5: The spatial distribution of the pressure for the porous system consisting of $8 \times 8 \times 8$ Argon atoms.



(a) The spatial distribution of the pressure at $t = 30$



(b) The spatial distribution of the pressure at $t = 40$

Figure 6: The spatial distribution of the pressure for the porous system consisting of $8 \times 8 \times 8$ Argon atoms.

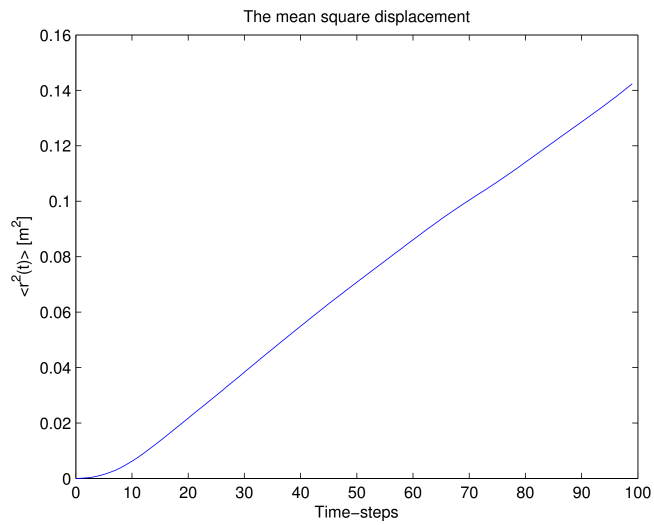


Figure 7: The displacement $\langle r^2(t)\rangle$ for the low density fluid in the porous medium consisting of $8 \times 8 \times 8$ Argon atoms.

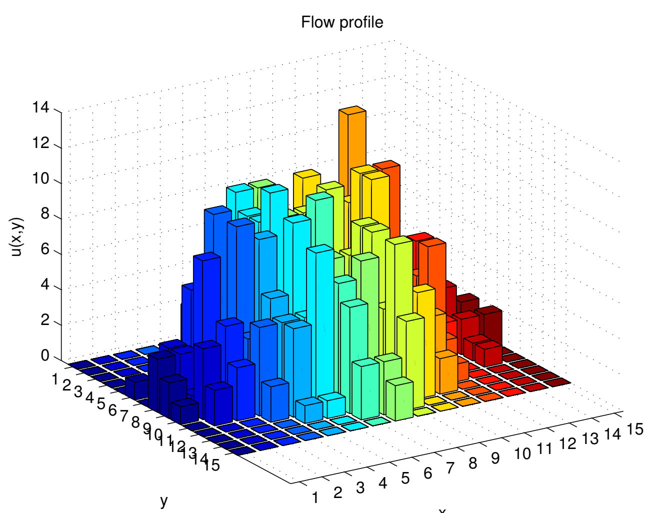


Figure 8: The flow profile in a cylindrical pore for a $8 \times 8 \times 8$ Argon system.

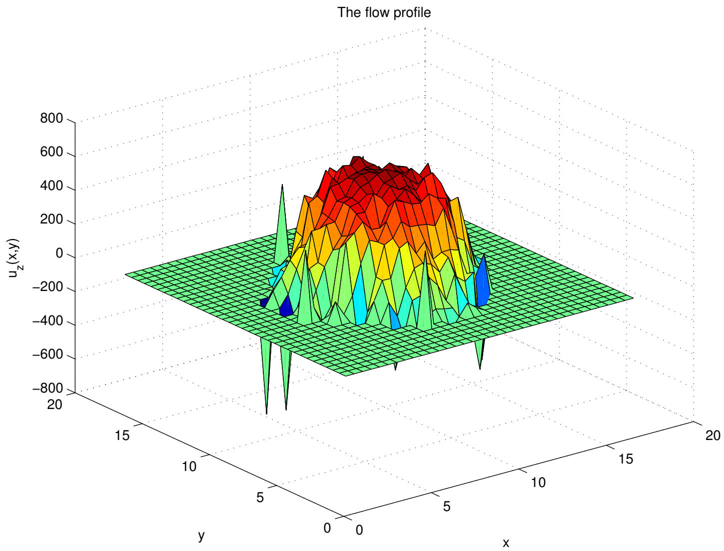


Figure 9: The flow profile in a cylindrical pore for a $8 \times 8 \times 8$ Argon system.

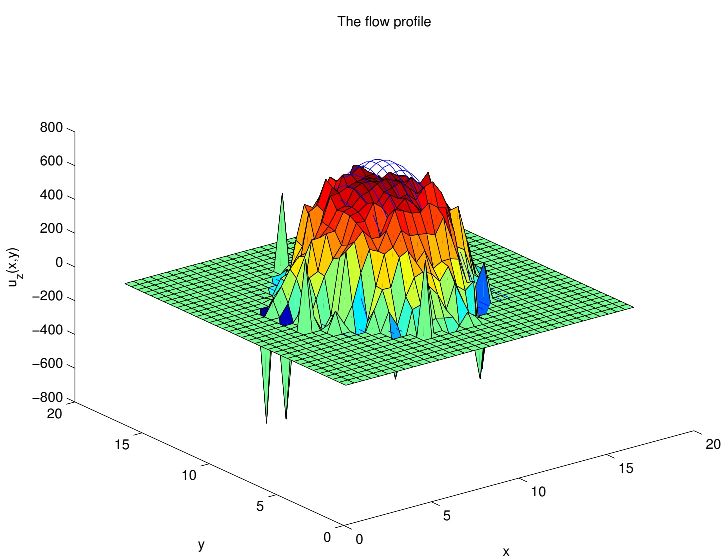


Figure 10: The flow profile in a cylindrical pore for a $8 \times 8 \times 8$ Argon system.