Project 2, FYS4460

Fredrik E Pettersen
f.e.pettersen@fys.uio.no

April 3, 2013

Contents

1 About the problem

The goal of this project is to model flow in a nanoporous material. For simplicity we will do this using the Lennard-Jones potential from project 1, and fix the positions of some of the Argon atoms.

2 The algorithm

The algorithm is in essence the same as in project 1 with some minor modifications. Since some of the Argon atoms are supposed to be fixed i space, we only need to calculate forces and possitions for the ones that are not fixed. Probably the most efficient way of doing this would be to make two separate lists of atoms in the program; one containing movable, and one containing immovable atoms. However implementing this would (I suspect) be a very demanding modification to my program from the first project, and so I have solved this by testing. If the atom is marked as immovable, no calculations are done. In this way I only had to add two lines to the force-part of the existing code, and everything worked as it should.

3 Points of progress

First of all we will make a cylinder with a radius of 2nm. This cylinder is shown in figure 1 where I have visualized only the stationary atoms.

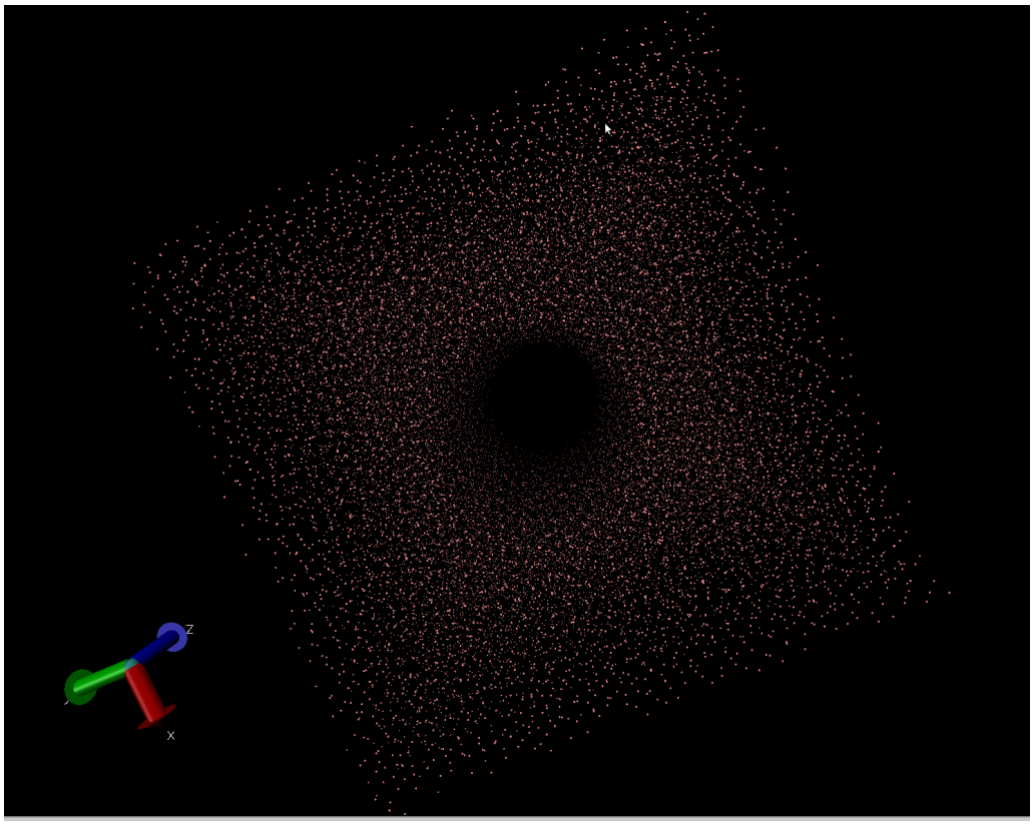
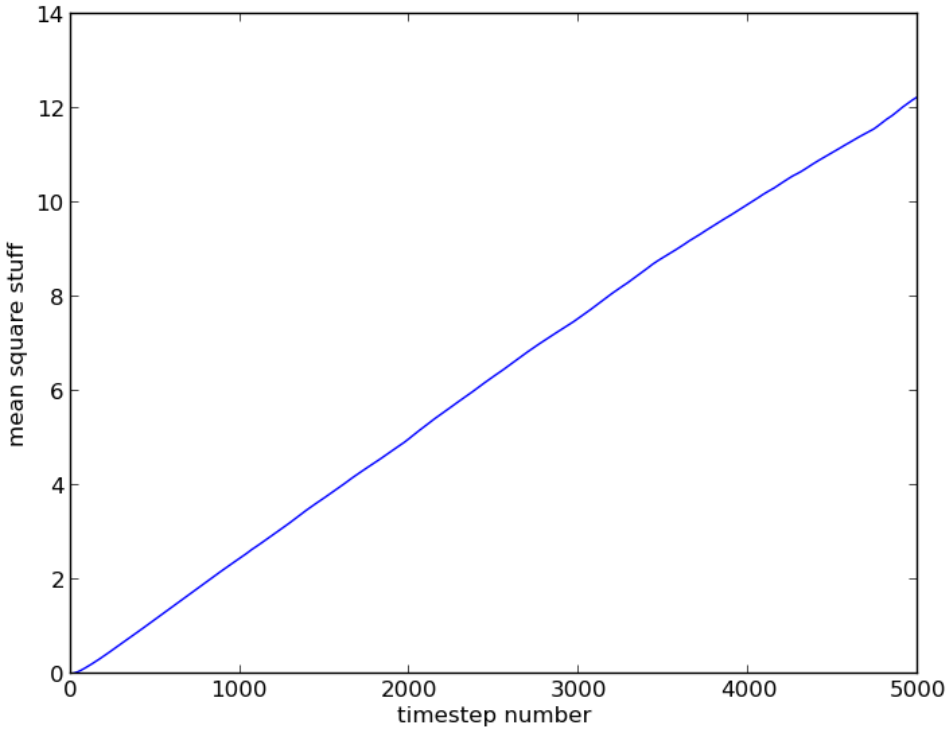


Figure 1: Cylinder with radius 2nm

Next we generate a matrix consisting of 20 spherical pores at random positions and with random radii ranging from 2nm to 3nm. The porosity of this system is 52.4% which I have measured simply by counting the number of atoms within the pores and dividing this by the total number of atoms. Compared to what we would expect from 20 non-overlapping spherical pores with uniformly drawn random radii ranging from 2 to 3nm which makes a volume of between $670nm^3$ and $2250nm^3$ making the porosity somewhere between 44.7% and 100% with an expectation value of ($\hat{r} = 2.5$) $\phi = 87\%$.
There should be quite a few other ways to measure the porosity of the generated matrix which proably are a bit more accurate than my approach. One could, for example, calculate the volume of each atom by drawing a line to all neighbouring atoms and at the middle of each line draw a normal plane. The volume of an atom is then the volume of the resulting figure, making the porosity of the system the ratio between the volume of movable atoms to the immovable ones.

We would now like to study a fluid at half the density. The way I interpret this we would like to keep the density of the "solid" the same. The only way I can think of which lets us do this is by removing half of the particles which are allowed to move. We do this by looping over the movable atoms and drawing a random (uniform) number. If it is less than one half, the atom is removed. This will generalize to more factors if it should be of interest.
Figure 3 shows $\langle r^2(t) \rangle$ for the low-density fluid in the nanoporous matrix without any external factors.



Darcy's law states that

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

inserting for $\rho = \frac{nm}{V}$ and $n = \frac{N}{V} \implies nV = N$ we obtain

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

From Newtons second law know that ma = F which in our case is F_x and so wa canreplace ρg by nF_x

4 Results

5 Stability and precision

6 Final comments