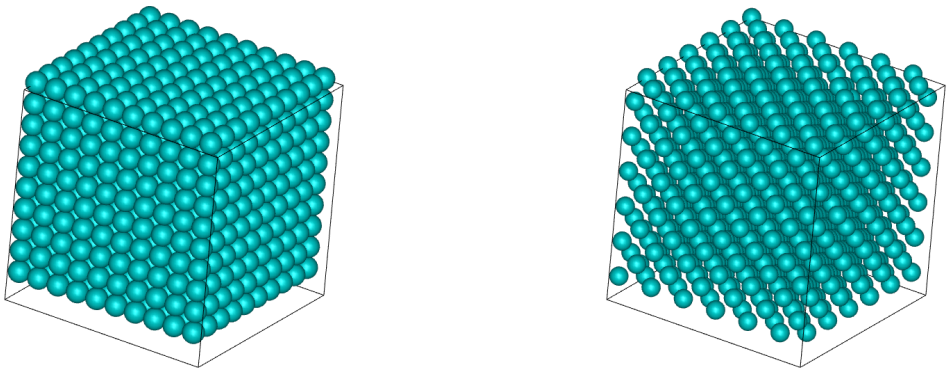
Modelling & Simulations
Monte Carlo simulation
of Hard spheres

Tom Niessen 3980820
Floris Jonkman 3943259

February 21, 2018



(a) **(b)**

Figure 1 – Figure (a) shows a cubic crystal configuration created in the first exercise. Figure (b) shows a face-centered cubic (ffc) crystal configuration created in third exercise.

Exercise 1 & 2: Cubic

In the first exercise we have written a program in C++ which creates a cubic lattice configuration and outputs a file. The result of the program is shown in Figure 1a. The code is sent with our assignment in a separate .cpp file.
In the second exercise we calculated the maximum volume fraction of a cubic lattice without any particle overlaps. The distance between two particles is exactly the lattice spacing: l. This means that the radius of a particle can be maximally $\frac{1}{2}l$, at which the particles do not overlap. In a cubic lattice configuration every lattice contains one particle. Therefore the volume in a lattice that is occupied by the particle is equal to:

$$V_{\text{particle,cc}} = \frac{4}{3}\pi\left(\frac{1}{2}l\right)^3 = \frac{1}{6}\pi l^3$$

The volume of the lattice and ratio between these two are respectively:

$$V_{\text{lattice}} = l \times l \times l = l^3$$

$$\frac{V_{\text{particle,cc}}}{V_{\text{lattice,cc}}} = \frac{1}{6}\pi\frac{l^3}{l^3} = \frac{1}{6}\pi \approx 0.52$$

This is the maximum volume fraction you can obtain using a cubic lattice configuration.

Exercise 3 & 4: Face-centered cubic (fcc)

Here we have done the same as in exercise 1, but now for a face-centered cubic (fcc) configuration. The result of our program is shown in Figure 1b. The code is sent with our assignment in a separate .cpp file.
In the fourth exercise we had also had to calculate the maximum volume fraction for fcc without any overlaps. In an ffc the distance between two particles is $\frac{1}{2}\sqrt{\frac{1}{2}l^2}$. This means that the radius of a particle can be maximally $\frac{1}{2}\sqrt{\frac{1}{2}l^2}$, at which the particles do not overlap. In a cubic lattice configuration every lattice contains four particles. So the volume of a particle has to be multiplied by four in order to get the particle volume in a ffc lattice. Hence the volume in a lattice that is occupied by the four particles is equal to:

$$V_{\text{particle,fcc}} = 4 \times \frac{4}{3}\pi\left(\frac{1}{2}\sqrt{\frac{1}{2}l^2}\right)^3 = \frac{\pi}{3\sqrt{2}}l^3$$

The volume of the lattice and ratio between these two are respectively:

$$V_{\text{lattice}} = l \times l \times l = l^3$$

$$\frac{V_{\text{particle,fcc}}}{V_{\text{lattice}}} = \frac{\pi}{3\sqrt{2}}\frac{l^3}{l^3} = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

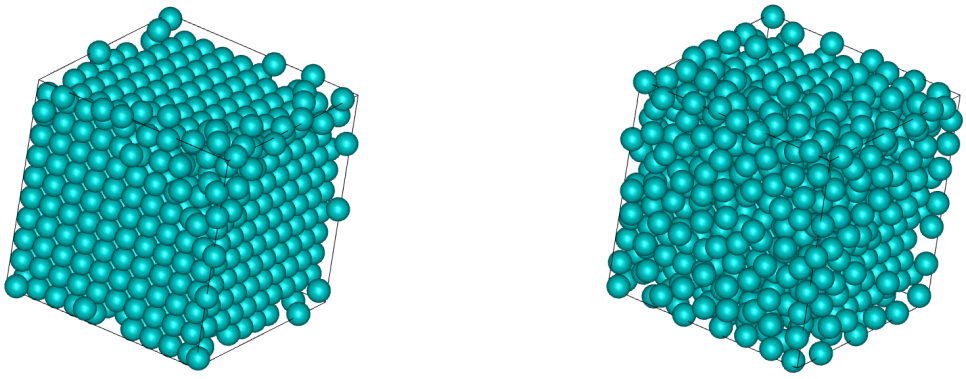
This is the maximum volume fraction you can obtain using a ffc lattice configuration.

Exercise 5 - 7

The program containing the code of exercises 5 to 7 can be found in a `.cpp` file, attached to our report. The code contains extensive commentary to explain what we have done and how.

Exercise 8

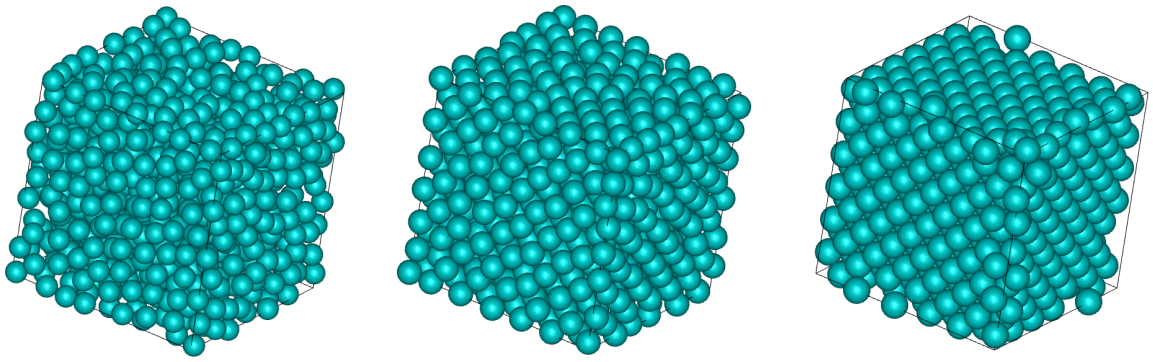
In figure 2a and fig 2b we see the results of our Monte-Carlo simulation for a cubic lattice for 200 and 2000 steps respectively. One can see that after some iterations the crystal structure disintegrates, we will eventually end up in chaos. The results of our simulations for fcc can be found in Exercise 9.



(a) **(b)**

Figure 2 – Visualization of Monte Carlo simulation of hard spheres. A cubic configuration is simulate for different steps. A figure (a) the simulation is ran for 200 steps, at figure (b) for 2000 steps.

Exercise 9



(a) **(b)** **(c)**

Figure 3 – Monte Carlo simulation of hard spheres, all with the same starting ffc configuration, particle size 1.0, maximum displacement parameter $\delta = 0.1$ and the number of Monte Carlo steps 5000. Figure (a) with a packing fraction of 0.5. Figure (b) with a packing fraction of 0.7. Figure (c) with a packing fraction of 0.8.

In this exercise we performed our Monte Carlo simulation starting with a ffc configuration. All with the same particle size 1.0, maximum displacement parameter $\delta = 0.1$ and number of Monte Carlo steps 5000. We have performed the simulation for different values of the packing fraction. The results of these simulations are shown in Figure 3. One can clearly see that at a packing fraction of 0.5 there is no structure left after 5000 steps. At a packing fraction of 0.9 the structure is still in intact. We estimate that the minimal packing fraction, for which the crystal structure stays intact, is around 0.7.