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Computer Simulations in Statistical Physics

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Problem set 4

Proseminar

The most naive way to model an atom or macromolecule in a computer simulation is using the hard sphere model. This model defines particles with diameter σ by its interaction potential $V(r)$ with other hard spheres,

$$V(r) = \begin{cases} 0 & r > \sigma \\ \infty & r \leq \sigma \end{cases} . \tag{1}$$

This potential just encodes that no overlap between hard spheres is allowed. Today you will learn that despite the very trivial nature of the model[1] the many-body physics is very rich. This precisely emphasizes the idea (and difficulty) of statistical physics: Very simple building blocks lead to complex phenomena in many-body systems.

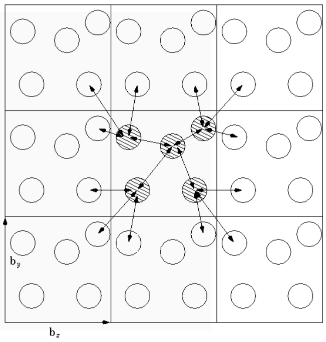
In the following exercises we will consider hard spheres of diameter $\sigma = 1$. They will be compressed into a cubic box with volume $V = L^3$, with box length L that is depending on the number of particles N and the packing fraction φ which is the only control parameter. The centres of mass of the particles are thus located at $\mathbf{r} = (x, y, z)$ with $x, y, z \in [-L/2, L/2]$. To avoid the introduction of boundaries[2] we use *periodic boundary conditions* (PBC).

[1] Due to the non-existent energy scale there is only one control parameter: the packing fraction φ. This parameter defines which percentage of the whole simulation box is covered by hard spheres.

[2] Boundaries would destroy the translational symmetry and thus introduce several complications to the system (e.g. layering at the walls). In a few weeks we might come back to this more advanced problem building up on the program you will write today.

This means that there is a direct connection between the sides of the boundaries, similar to the case you learned last week for the Ising model. Every particle will only interact with the closest copy of the other particles (see picture on the right). For example, the upper right grey particle interacts with the white copies of the other particles in the box because they are closer than their grey counterparts. In the following you will find pseudocode that realizes periodic boundary conditions and calculates the distance r between two particles, labelled 1 and 2.

```
rx = x1 - x2
ry = y1 - y2
rz = z1 - z2
if (rx > L/2) rx -= L
if (rx < -L/2) rx += L
if (ry > L/2) ry -= L
if (ry < -L/2) ry += L
if (rz > L/2) rz -= L
if (rz < -L/2) rz += L
r = sqrt(rx*rx + ry*ry + rz*rz)
```



Proseminar

Problem 4.1 *Initialization and Visualization*

To perform computer simulations the first task is the initialization and visualization of the data.

Here, we will use lattice packing for the initialization of a box with packing fraction φ. In lattice packing the particles are placed on a (simple-cubic) lattice. To obtain the correct packing fraction follow the following recipe:

- for simplicity take $N = n^3$;
- place the N particles on a cubic lattice with lattice constant σ. This lattice will have a volume $V' = (L')^3$ with $L' = n\sigma$;
- Shift the center of mass of the entire system in $\mathbf{r} = (0, 0, 0)$;
- Perform a scale transformation on the entire system to match the correct packing fraction.

a) What is the highest packing you can achieve using this procedure? Is there a way to get to even higher packing? What is the maximal possible packing fraction you can achieve with monodisperse hard spheres (monodisperse means that all particles have the same diameter)?

b) Setting $N = 64$ and $\sigma = 1$, create a configuration with $\varphi = 0.2$ and one with $\varphi = 0.5$ and visualize them using the python script “python_visualize_spheres.py” (see project folder).

Problem 4.2 *Importance Sampling: The Metropolis Algorithm*

We now want to perform computer simulations, starting from the initial configuration created in Problem 4.1. Therefore, we have to implement the Metropolis algorithm (see lecture notes). In our case every “Monte Carlo (MC) move” consists of N move attempts. In each attempt a random particle is shifted in a random direction to a distance δ. If the move leads to a particle overlap it will be rejected, otherwise it will be accepted.

a) Implement the Metropolis algorithm into your simulation program.

b) Perform computer simulations with packing fraction $\varphi = 0.2$. Always monitor the acceptance ratio and adapt the step size δ accordingly[3].

c) Monitor the particle averaged minimum distance between particles $\langle x_{\min} \rangle$[4] (you should calculate it every 10-100 MC moves). Observe the equilibration process starting from different initial configurations at $\varphi = 0.2$, $\varphi = 0.4$ and $\varphi = 0.52$. What do you observe?

[3] For your projects, please note that this optimization has to be done in the first N_{eq} moves, before performing measurements on your system.

[4] $\langle x_{\min} \rangle = \frac{1}{N} \sum_i^N \min\limits_{j \neq i} \{r_{ij}\}$, $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$