Exercise 1. Linked-Cell Method

Goal: As you have seen in the last exercise, in a Molecular Dynamics simulation the most time-consuming part is the calculation of the total force on a particle. However, when the interaction between the particles is short-range, it is not necessary to consider the interaction with particles far away from the particle for which the total force is calculated. In the Linked-Cell Method one can use this fact to eliminate the unnecessary computations by dividing the system into smaller regions such that the particles from one region can only interact with the particles in the same or neighboring (next-nearest neighbors) regions.

Task: *Implement the* `Linked-Cell Method` *as described in the lecture notes. How many particles can you simulate?*

Hint: Adapt your code from last week's exercise sheet.

Solution. Since we simulate a system of N particles in a cubic box, we divide the system into smaller cubic regions of size $M = r_c$ where $r_c = 2.5\sigma$ is the interaction range (cut-off of the interaction potential) like in last week's exercise. As described in the lecture notes, we use the arrays `FIRST` and `LIST` to store which particle belongs to which cell. The `Linked-Cell Method` allows us to reduce the complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$. For small systems (a few hundred particles) this might be slower than the original algorithm but for large systems this speed-up is very important and the saved computation time can be enormous. However, note that in the example code that we provide you we did not implement a local update scheme for the arrays `FIRST` and `LIST` as suggested in the lecture notes.