Computational Statistical Physics
Exercise sheet 08

FS 2020
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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.