

Linked-Cell Method

As you saw in the last exercise, the most time-consuming part of a Molecular Dynamics simulation is the calculation of the total force on a particle. However, when the interaction between 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 uses this fact to eliminate unnecessary computations by dividing the system into smaller regions, such that particles from one region only interact with particles in the same or neighbouring (next-nearest neighbours) regions.

Implement the Linked-Cell Method as described in the lecture. How many particles can you simulate?

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