Report for Exercise 08

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May 3, 2022

1 Task 1

For this task I implemented the linked cell method for the 3d molecular dynamics simulation using a Verlet scheme. In Figure 1 one can see the run times plotted over the Number of particles both for the linked-cell Verlet and for the normal Verlet from task 07. I think it is interesting that the linked cell method has better run-time for 10 and more molecules, whereas the book "Computational Statistical Physics" by Lucas Böttcher says that linked cell only makes sense for more then a few hundred particles. I assume that python is the reason the linked cell method performes so good in my simulation. Also one can observe that for bigger numbers of molecules the run-time of the linked-cell method does not grow linearly anymore. This could be because I have not updated the box size for bigger numbers of molecules.

To proof this I plotted the run-times of the linked cell method for constant box size and for box size increased linearly over the number of molecules. The plot can be found in Figure 2.

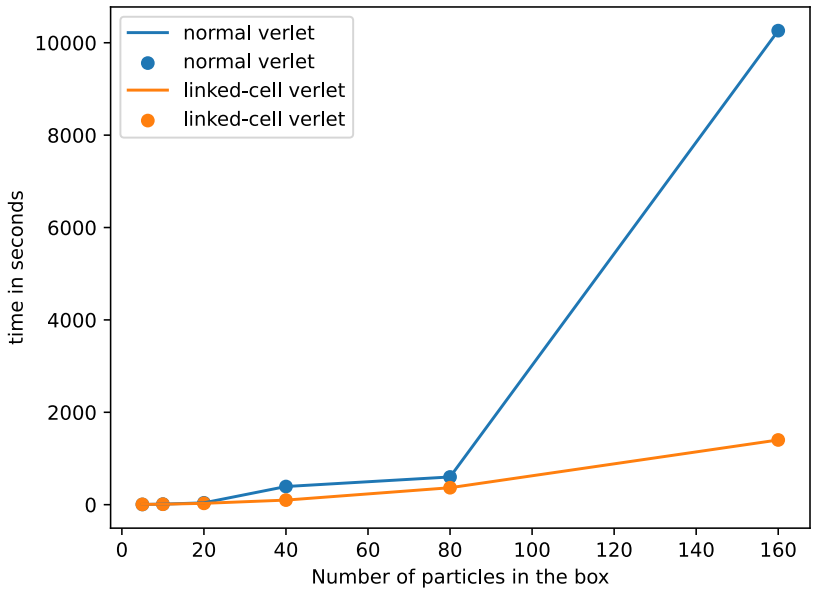

Figure 1: Run-time over number of molecules for the normal Verlet simulation and linked cell Verlet.

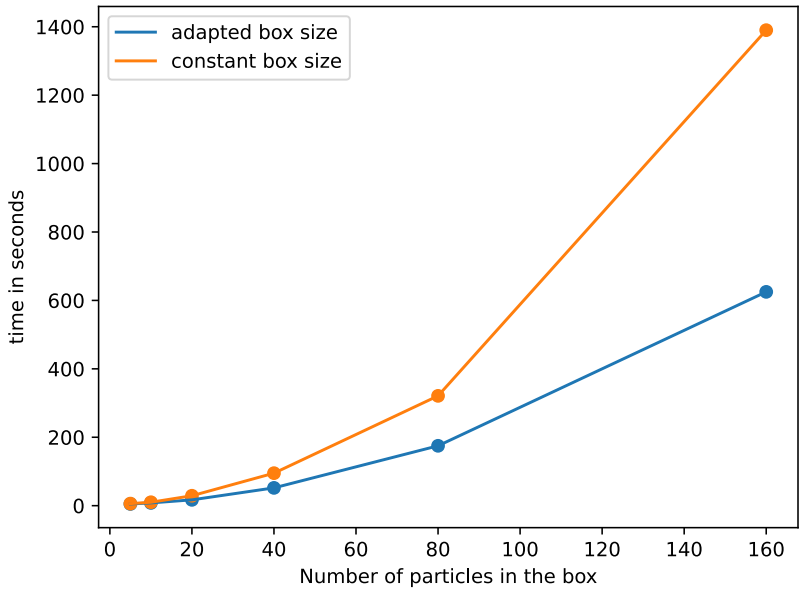

Figure 2: Run-time over number of molecules for the linked cell simulation with constant box size and linearly increasing box size.