Molecular Dynamics Exercise I: Introduction to Molecular Dynamics

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1 Introduction and Procedure

The aim of this exercise was the MD simulation of 4 given particle systems with 1000 C dimers each and to test the simulation stability in dependence of an increasing time step dt. The weight of the atoms in the systems was 2,4,6 and 12 Daltons respectievely. For the MD simulation the software GROMACS was used.
For each of the particle systems a physically possible structure was found by minimising the energy. Using this structure, the given MD simulation was started with a selected time step dt. After this the kinetic-, potential- and total energy were extracted. When the energy curves behaved stable, the time step was increased by 0.001 ps. Once an exploding or energy conservation violating solution was found, the time step was varied by 0.0005 ps to find an unstable or exploding solution respectively.
The simulations of the particle systems with larger weight were started with the time step that lead to energy conservation violating behaviour in the lighter system.

2 Simulation Results

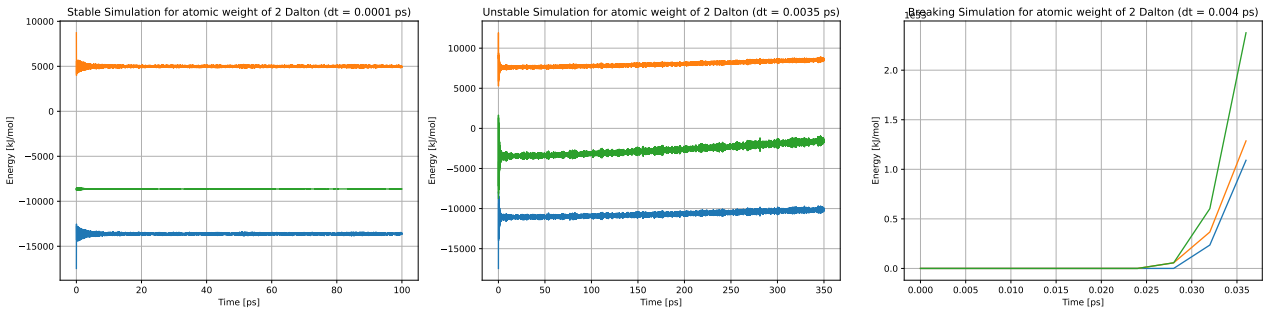

Figure 1: Results for the particle system with atom weight 2 Dalton.

For the particle weight of 2 Dalton the simulation was started with the recommended time step dt = 0.001 ps, leading to stable energy trajectories. The simulation starts to become unstable around a time step dt = 0.0035 ps and explodes shortly after at dt = 0.004 ps as can be seen in figure 1. Based on this results one should use a time step dt $\approx$ 0.003 ps for simulations with this system. In this way one can simulate T = 300 ps and ensure energy conservation. The results for the other systems are listed in the table below. Furthermore, the energy trajectories are provided (Figures 2, 3 and 4).

	time step			
atom weight	Stable sim [ps]	Unstable sim [ps]	Breaking sim [ps]	Recommended [ps]
4	0.0035	0.005	0.0055	≈ 0.004
6	0.005	0.006	0.0065	≈ 0.005
12	0.006	0.008	0.00925	≈ 0.007

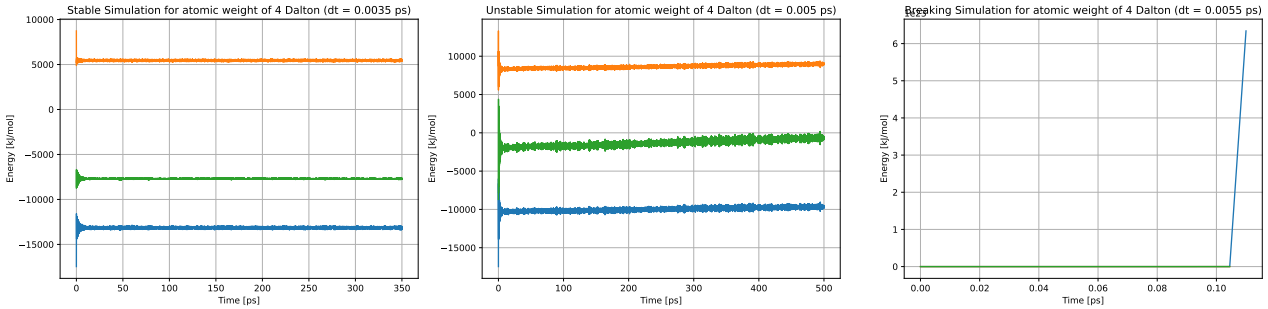

Figure 2: Results for the particle system with atom weight 4 Dalton.

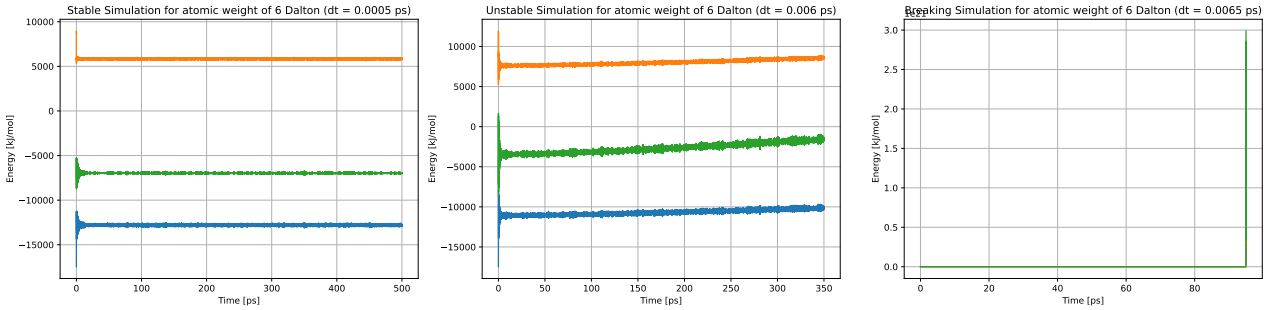

Figure 3: Results for the particle system with atom weight 6 Dalton.

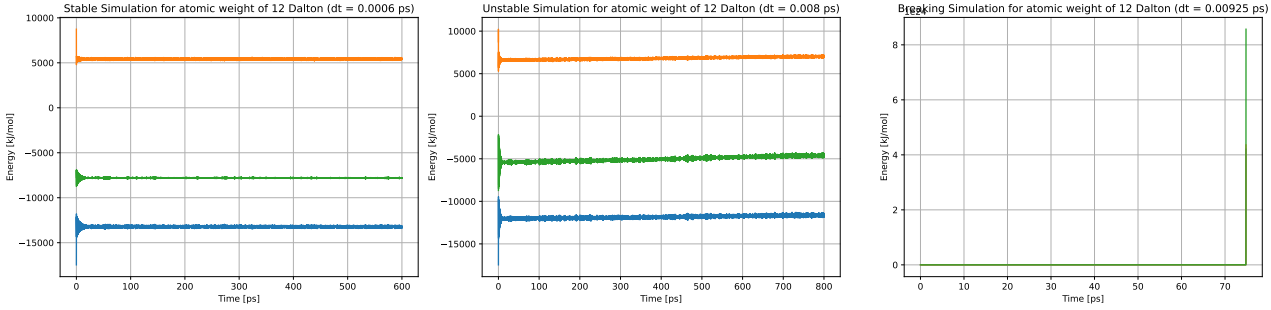

Figure 4: Results for the particle system with atom weight 12 Dalton.

3 Conclusion

From the results presented in the previous section, one can clearly see that the increase in mass of the atoms making up the molecules allows for larger time steps in the integration of the equations of motion. The increase in total energy (and later the exploding of the simulation) means that the atoms have left their physically possible configurations. This is due to the oscillation frequencies which are dependent on the mass of particles. For lighter particles the short period times mean that for a too large time step the atoms overshoot their physically possible

amplitude and end up unphysically close to each other. At this point the short range repulsion from the Van-der-Waals Forces causes the atoms to break apart, leading to the exploding of the energy and hence the breaking of the simulation. The lower frequency of the molecules with higher mass means that this effect only occurs at larger time steps, enabling longer simulation intervals.