Molecular Dynamics Exercise I: Introduction to Molecular Dynamics

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December 23, 2024

1 Introduction and Procedure

In this exercise the effects of an increased time step and an increase in mass of atoms on the stability of molecular dynamics simulations was explored. For this four systems consisting of 1000 dimers each with the weight of the atoms being 2, 4, 6 and 12 Daltons respectively were simulated at several time steps. For each the time step leading to a diverging energy was determined. The MD simulations were conducted with the free software GROMACS.

First an energy minimization was run on each of the particle systems to find a physically likely structure. Using this structure, the given MD simulation was started with a selected time step Δt. 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.

To save computational time the simulations of the particle systems with larger atomic weight were started with the time step that lead to energy conservation violating behaviour in the next lighter system.

2 Simulation Results

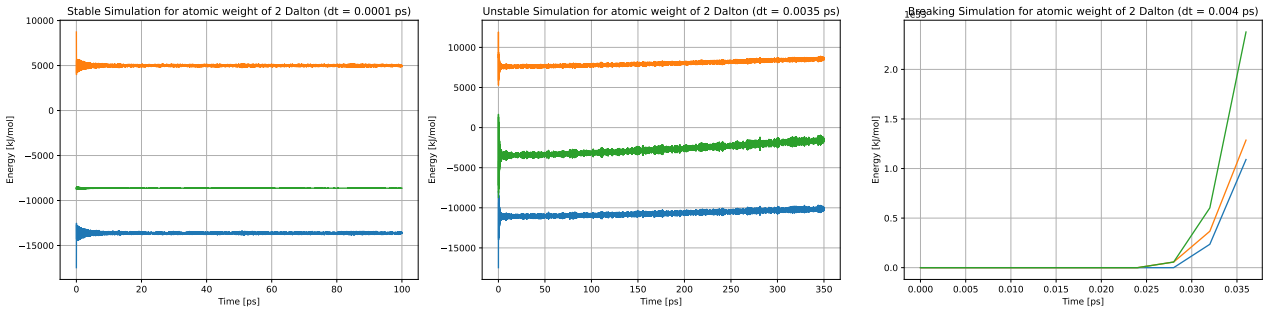

Figure 1: Results for the particle system with atom weight 2 Dalton.

For the particle weight of 2 Dalton the simulation was started with the recommended time step $\Delta t = 0.001$ ps (1 fs), leading to stable energy trajectories. The simulation starts to become unstable around a time step dt = 0.0035 ps and explodes at $\Delta t = 0.004$ ps. This behviour can be see in the figure 1 above. Based on these results one should use a time step $\Delta t \approx 0.003$ ps

for simulations of this system. This way, energy conservation is ensured and the best ratio of trajectory duration and computational cost is achieved. The results for the other systems are listed in the table. Furthermore, plots of the kinetic. potential and overall energy are provided (Figures 2, 3 and 4).

atom weight [u]	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

Table 1: Time step limits for the systems with particle masses 4 u, 6 u and 12 u.

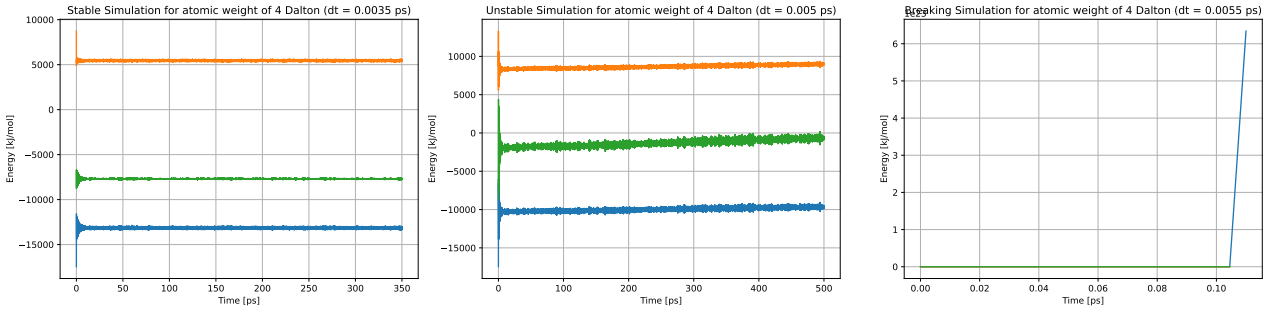

Figure 2: Results for the particle system with atom weight 4 Dalton.

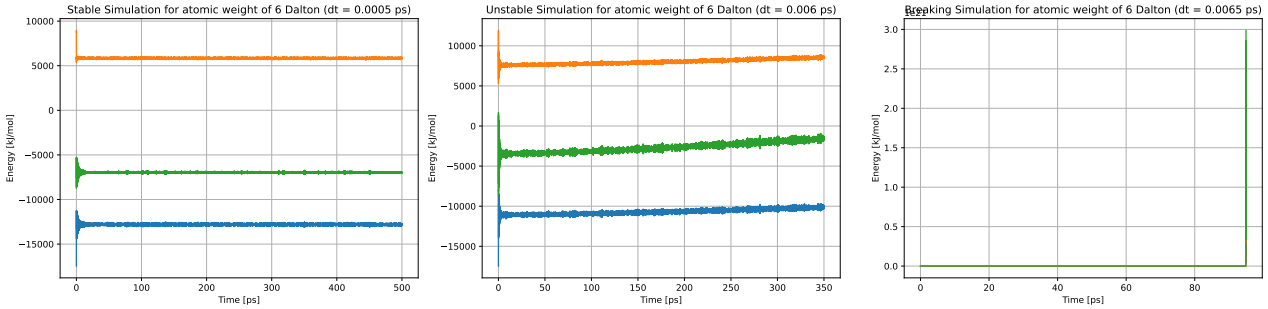

Figure 3: Results for the particle system with atom weight 6 Dalton.

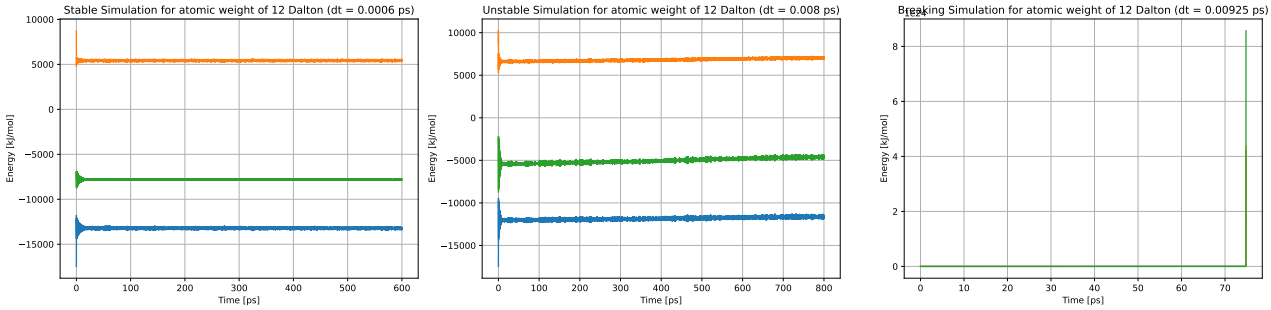

Figure 4: Results for the particle system with atom weight 12 Dalton.

3 Conclusion

From the results presented in the previous section, one can clearly see that the increase in mass of the atoms forming the dimers 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 periods which are dependent on the mass of particles.

$$T = 2\pi \left(\frac{m}{k} \right)^{\frac{1}{2}} \tag{1}$$

Here k is the force constant of the harmonic potential usually used to model electronic bonds between two atoms. In practice, the short period time of light particles means that for a large time step the atoms overshoot their physically possible amplitude and end up unphysically close to each other. At this point, the short range repulsive part of 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. Molecules composed of atoms of larger mass means can tolerate larger time steps before this effect occurs, enabling longer simulation intervals for the same number of steps.