Time-step	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
Distance at end time	$3.03319 \cdot 10^{-8}$	$1.13779 \cdot 10^{-8}$	$7.3358 \cdot 10^{-9}$	$6.79042 \cdot 10^{-9}$	$6.7332 \cdot 10^{-9}$

10^{-6}	10^{-7}	10^{-8}
$6.7274 \cdot 10^{-9}$	$6.7269 \cdot 10^{-9}$	$6.7269 \cdot 10^{-9}$

Figure 3: Time-step and distances at end time.

Figure 1 presents the results of 8 different simulations of our Lennard-Jones implementation, for time steps $\Delta t \in \{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}\}$.

For all 8 simulations we see that for $0 \leq time \leq 4100$ all simulations produce near-identical results (hence only one line is visible on the graph) and the two molecules gradually get closer to each other. At $time = 4100$ the molecules reach the minimum distance ($\approx 10^{-9}$), and as a result of our force model the molecules begin to get further away from each other. We see that in the simulation with time step 10^{-1} the two molecules begin to diverge away from one another. This is a result of the large time step causing the spike in force to have more of an impact on the simulation. We see similar behaviour in the simulations with 10^{-2} and 10^{-3}, however due to the smaller time steps thid is on a much smaller scale. We see that time steps $\{10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}\}$ produce very similar distances throughout the entire simulation, these time stepping schemes are numerically stable throughout the entire simulation. Figure 1 exhibits the property of stiffness in our algorithm and shows that our method for solving the equation is only numerically stable for sufficiently small time steps (i.e. $\Delta t \leq 10^{-3}$). We see in both Figure 1 and Figure 2 that unless the step size is sufficiently small $\Delta t \approx 10^{-4}$ the distances yielded by the algorithm vary a lot, and small changes can make a huge impact on the overall result for time stepping schemes with larger time steps.

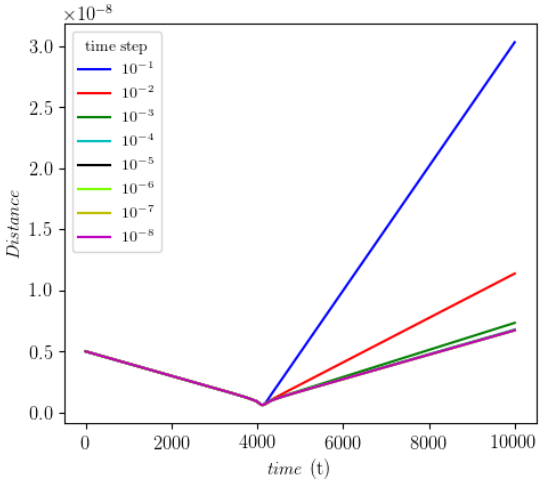

Figure 1: The distance between the particles for $0 \leq time \leq 10000$, for 8 simulations with different time steps.

Figure 2 and Figure 3 presents the end time distances of the simulation for each time step in a more clear manner. From this it is clear to see that as we decrease the time step the end-time distance converges to a value, this is illustrated by (approximately) constant line from time step 10^{-4} onwards. Should the value it converges to be the analytical solution then our scheme is consistent. If we take the formula $|F^{(i+1)} - F^{(i)}| \leq C|F^{(i)} - F^{(i-1)}|^p$ with $p = 1$ fixed and compute C, we see that for each set of $F^{(i-1)}, F^{(i)}$ and $F^{(i+1)}$ we have $C \approx 0.1$. This is the experimental method of determining the order and thus it's clear that the solution converges linearly (with order 1) - otherwise stated with order 1.

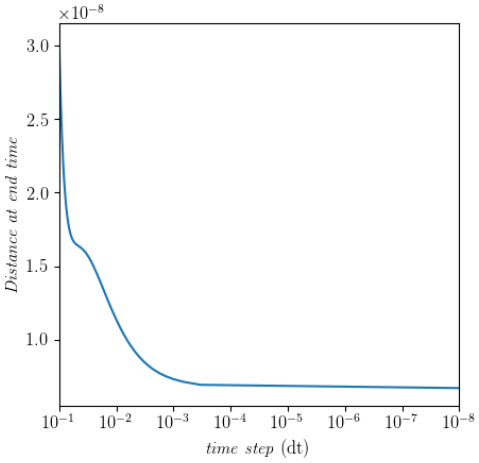

Figure 2: The end time distance of each of the simulations.