Exercise 1. Interacting particles in a box

Goal: This week's exercise is about simulating a system of N interacting particles in a box using the Verlet scheme.

Note: *The code of this exercise will be the basis for further improvements and modifications in the following exercises. Therefore, please make sure that it is easily readable and well-structured.*

Consider a system of N point particles (in a box of length L with periodic boundary conditions) that interact via the Lennard-Jones potential

$$V(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6}\right]$$

with each other. The total Hamiltonian of the system is given by

$$H = \frac{1}{2}\sum_i \boldsymbol{v}_i^2 + \frac{1}{2}\sum_{i\neq j} V(|\boldsymbol{r}_i - \boldsymbol{r}_j|).$$

Task 1: *Simulate the system by using the Verlet scheme.*

Hint: Use sufficiently small time steps and a cutoff length $r_c = 2.5$ for the Lennard-Jones potential.

Task 2: *Investigate the influence of the choice of the time step size.*

Task 3: *Measure the energy of the system as well as its fluctuations. Is the energy conserved?*

Visualization of the results: *For visualizing the particles you have different options. You can simply use a graphical tool (e.g. matplotlib or gnuplot) which reads in the coordinates for a given time step. Another possibility would be to use either vmd (https://www.ks.uiuc.edu/Research/vmd/) or paraview (https://www.paraview.org/) to visualize the dynamics and create movies.*

If you want to use paraview then the following information might help you to get started. To be able to visualize your simulation you may use the provided `vtktools.py` *and* `convert_to_paraview.py` *to bring your computed data into an appropriate shape for paraview.*

Once your simulation is finished you can go over to paraview and follow the steps below:

1. *Load the data files.*

   - *Open paraview.*
   - *Go to "File" → "Open" and choose the group* `MD..vtu` *in the folder* `simu`.
   - *Click "Apply" in the "Properties" window.*

2. *Display the particles.*

   - *Click "MD*" in the "Pipeline Browser" window.*
   - *Find the "Glyph" symbol in the toolbar and click it.*
   - *In the "Properties" window set "Glyph Type" → "Sphere", "Vectors" → "Points", "Scale Mode" → "Scalar", "Scale Factor" → "0.5", "Glyph Mode" → "All Points" and click "Apply".*

3. *Add the forces.*

Solution. For the simple molecular dynamics implementation of N particles in a box with periodic boundary conditions, different time step sizes and initial velocities were studied. If the time steps are too big it might happen that some events cannot be resolved properly. Thus, depending on the number of particles per volume and their velocities it has to be chosen small enough to deliver reliable results. An example simulation can be found in the file MD.mp4. A screenshot is shown in Fig. .
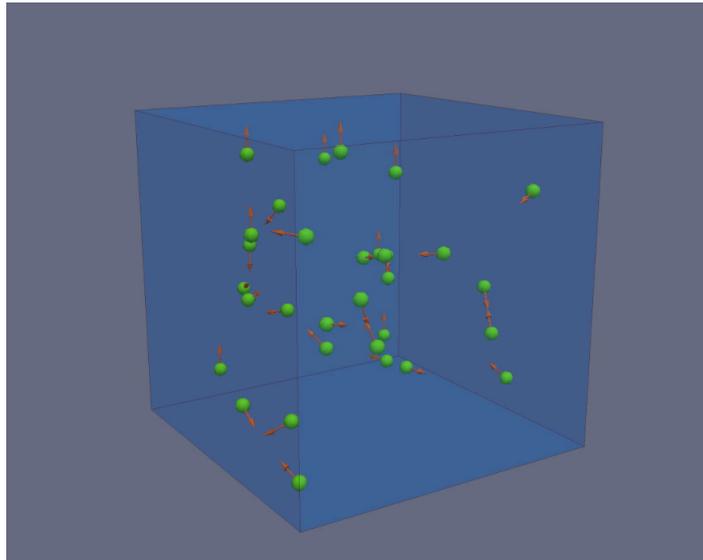
Figure 1: Screenshot of a MD simulation of $N = 30$ particles in a box.

A typical energy curve with its fluctuations is shown in Fig. .
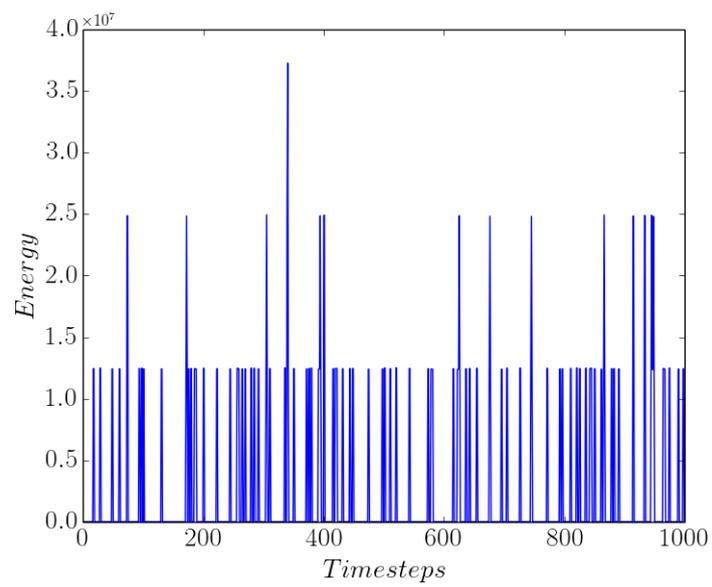
Figure 2: The total system energy for the simple MD implementation.