Simple molecular dynamics

Goal: Getting started with molecular dynamics simulations with a system of N interacting particles in a box using the Verlet scheme.

Hint: Having an effort for a well-structured and easily readable code for this exercise would be a good strategy, because this will be the basis for further modifications in the following exercises.

Consider a system of N identical classical point particles in a 3-dimensional square box of side-length L with periodic boundary conditions. We assume the particles interact pairwise via the Lennard-Jones potential[1]

$$V(r) = 4\left(r^{-12} - r^{-6}\right), \tag{1}$$

where r is the separation between two particles. The full Hamiltonian of the system is then given by

$$H = \frac{1}{2m}\sum_{i=1}^{N} v_i^2 + \frac{1}{2}\sum_{i\neq j} V\left(|\vec{r}_i - \vec{r}_j|\right). \tag{2}$$

Task 1: Simulate this system using the Verlet method. Save the particle coordinates and forces at each time step to visualise the dynamics later on.

Hint: Use sufficiently small steps to discretise time. Moreover you can define a cut-off radius $r_c = 2.5$ for the potential to avoid wasting computation time for negligible pairwise interactions at large distances.

Task 2: Measure the time evolution of the total energy and its fluctuations. Is the energy conserved?

Task 3: Investigate the influence of the time discretisation size on your results.

Visualising your simulation. You have multiple options to visualise the dynamics of the many-particle system. First, you can simply use a generic library like `matplotlib` or `gnuplot`. Another option is to use more specialised tools for visualising molecular dynamics simulations such as `vmd` or `paraview`. In the following we provide some information to help you get started in case you want to use `paraview`, which you can download from `https://www.paraview.org/download/`.

Once your simulation is finished, follow the steps below:

1. Bring your dataset for the coordinates and velocities into an appropriate shape for `paraview` using the provided script `vtktools.py`.
2. Go over to `paraview` and load the data:

[1] Models electronic molecular interactions by accounting for (short-distance) Pauli exclusion and long-range van der Waals attractive forces.

Go to `File` → `Open` and choose the group `MD..vtu` in the folder `simu`.

Click `Apply` in the `Properties` window.

3. 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`, `Orientation Array` → `Points`, `Scale Factor` → `0.5`, `Glyph Mode` → `All Points` and click `Apply`.

4. Display the forces:

   Click again `MD*` in the `Pipeline Browser` window and add another `Glyph`.

   In the `Properties` window set `Glyph Type` → `Arrow`, `Orientation Array` → `Forces`, `Scale Factor` → `0.75`, `Glyph Mode` → `All Points` and click `Apply`.

5. Add a box:

   Go to `Sources` → `Geometric Shapes` → `Box` and adjust it properly. *E.g.*, in the case where $L = 10$, set `X Length` → `10`, `Y Length` → `10`, `Z Length` → `10` and `Center` → `5 5 5`; click `Apply`.

   Set `Opacity` → `0.2`.

6. Click the `Play` symbol in the toolbar. (Note that you might need to zoom out and/or move around in the coordinate system to see something.)

You can save the simulation movie by going to `File` → `Save Animation` and following the dialogue therein.