Computational Physics SuSe 2023
3. Exercise Sheet

Handing out: 28.04.2023 Prof. H. Jelger Risselada
Submission: 12.05.2023 12 pm

Exercise 0: Comprehension questions 0 Points

1) What should you be aware of, initializing an MD-simulation? Why is it necessary?
Tipp: What would happen if two particles would occupy exactly the same position?

2) What is described by the pair correlation function? Which properties does this function have and what does it tell you about your system?

Exercise 1: 2D Lennard-Jones-Fluid 40 Points

Molecular dynamics simulations are an essential tool in numerical physics for describing the behavior of of larger quantities of atoms or molecules, if the potential of their interaction is known. In this task, such a molecular dynamics simulation shall now be exemplified for a simple bath of uncharged particles in two dimensions. The interaction of such particles can be described by the Lennard-Jones potential.

Implement a molecular dynamics simulation for N identical particles of mass $m = 1$ with a pairwise Lennard-Jones interaction.

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

Set $\epsilon = \sigma = 1$, meaning lengths are given in units of σ and energies, as well as $k_\mathrm{B}T$ in units of ε. Use periodic boundary conditions in a System of size $A = L \times L$. Use a cutoff radius of $r_\mathrm{c} = L/2$ to determine the forces. Then use the Verlet algorithm with time steps of $h = 0.01$ (smaller time steps might be necessary for higher temperatures) as your integrator.
NOTE: A MD-simulation is a bigger project build up of several modules (like integrator, thermostat, etc.). That given, it might be helpful to do object orientated programming for this exercise. To help you with that, we provide you a template for python and C++. This, however, is just a recommendation and not mandatory for successfully completing this task.

a) Initialization:
To start off, take a square box of length $L = 2n\sigma$ and fill it with $N = n^2$ particles on equidistant positions. Choose your starting velocities such, that $\sum_{i=1}^{N} \vec{v}_i(0) = 0$, so that your center of mass is stationary. Write your program in such a manner, that you are able to rescale velocities to set your starting temperature to $T(t = 0)$.
Note: For random number generation, you are allowed to use already existing random number generators like f.e. `<random>` in C++:

```
#include<random>
mt19937 rnd;
uniform_real_distribution<> dist(0, 1);
random_number = dist(rnd);
```

b) Measurement/Equilibration:
Start at $T(0) = 1$ for $n = 4, 8, 16$. Calculate your center of mass velocity $\frac{1}{N}\sum_{i=1}^{N} \vec{v}_i(t)$ in dependence of time. Calculate the temperature $T(t)$ in dependence of time. Calculate the potential $E_\mathrm{pot}(t) = \sum_{i<j-1}^{N} V(|\vec{r}_i - \vec{r}_j|)$ as well as the kinetic energy $E_\mathrm{kin}(t) = \sum_{i=1}^{N} \frac{1}{2}\vec{v}_i^2$ as functions of

time. How long does it take for your System to equilibrate?

c) Measurement:
After the equilibration is done, you can now measure the temperature T and the pair correlation function $g(r)$. To do so, start to average over your system for 10^4 to 10^6 time steps (depending on how long you are willing to wait).
Do these measurements for $n = 8$ at three different starting temperatures $T(0) = 1$, $T(0) = 0.01$ and $T(0) = 100$. Which phases do you notice?

d) Thermostat:
Now implement an isokinetic thermostat for your MD-simulation and couple it to your System to keep a constant temperature. What does now happen for $T = 0.01$? Look at the potential, kinetic and overall energy during equilibration and measure $g(r)$ in the newly equilibrated system. It might also be interesting to look at snapshots of your system.

e) Physical and Chemical Systems **(Bonus: 5 Points)**

- Which quantities are kept constant during your simulation (after turning on your thermostat)?
- Which thermodynamic ensemble is represented by that?
- You are using an isokinetic thermostat for your system. Is this kind of thermostat physically accurate? If not, name a physically accurate alternative.
- A chemist asks you to do a MD-simulation on a chemical solution. In which way might such a system differ from the ensemble we considered so far? If you have to keep different quantities constant, name a way to do so for your simulation.
- Which further potential should also be considered for a chemical solution (f.e. NaCl in water)?