Universität Freiburg – Institut für Physik
Applied Theoretical Physics
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Freiburg, 3.5.2021
Due: 10.5.2021

Exercise 2 for '*Computational Physics - Material Science*', SoSe 2021
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Please provide a well documented submission of your solution. Your submission should include

- A pdf file containing the solution to the questions with the corresponding equations that are implemented in your codes. Figures must contain axis titles with corresponding units and a caption.
- The source code should be commented, and the equations given in the pdf file have to be referenced in the source code.
- There is no need to provide the trajectory files.
- In case your code is not working properly, please provide a description of the debugging attempts you did.

Exercise 2.1: LJ fluid-1: microcanonical ensemble

The Lennard-Jones (LJ) 6-12 interaction potential between two atoms is given by

$$U_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

where ϵ is the *well depth* of the potential, σ is the sum of their van der Waals radii, and r is the inter-particle separation. The objective of this exercise is to implement a basic MD code that computes the trajectory of a collection of N atoms interacting through the LJ potential in the microcanonical (NVE) ensemble, where V is the box volume and E the total system energy.

To allow each user to choose 'real' or 'natural' units based on personal preference, the following questions are phrased in general terms. At the end of the exercise, values for the various quantities are defined in the 'real' units. If real units are used, all output must be provided in the **SI units**.

a) Consider a cubic simulation box with dimension $L = p\sigma$ along each direction containing $N = n^3$ atoms. The cubic simulation box is the region of space bounded by $[0 \leq x < L; 0 \leq y < L; 0 \leq z < L]$, and the atoms are initially distributed on a cubic lattice with a lattice parameter, a_{lat}, bounded by the simulation box. Implement such a geometry with $n = 4$ and a number density $\rho = N/V = 0.1\sigma^{-3}$. Provide a snapshot of the initial geometry. What are the relations between p, n, ρ, and a_{lat} that need to be implemented in your code.

b) Assign randomly initial component velocities (v_{x0}, v_{y0}, v_{z0}) to each atoms, such that the initial temperature of the system is T (provided below).
Hint:
   - *Assign initial component velocities randomly in range* (-1,1).

- *Shift all velocities by the mean to cancel the linear momentum of the system (you should have*

$$\sum_{i=1}^{N} v_{x0}^{i} = \sum_{i=1}^{N} v_{y0}^{i} = \sum_{i=1}^{N} v_{z0}^{i} = 0$$

  after shift).

- *Rescale the velocities to achieve the desired temperature T.*

c) Implement periodic boundary conditions (PBC) to compute the shortest distances between the atoms following the minimum image convention.

d) The force between two atoms interacting through a LJ potential, $U_{LJ}(r)$, is given by $\vec{F}_{LJ}(r) = -\nabla U_{LJ}(r)$. Owing to the *short-range* nature of the LJ interaction, two atoms i and j interact with each other only if the distance between them, r_{ij}, is lower than a cutoff distance, r_{cut}. To cancel the interaction between atoms i and j for $r_{ij} \geq r_{cut}$, you should shift the interatomic potential by $U_{LJ}(r = r_{cut})$, such that $U(r) = U_{LJ}(r) + U_{LJ}(r = r_{cut})$ is the effective interacting potential between atoms i and j. In this exercise, $r_{cut} = 2.5\sigma$. Implement a routine that calculates the components of the force $\vec{F}_{LJ}(r)$ on atom i due to its interaction with atom j.

Using PBC along each dimension and the Velocity-Verlet time integration scheme, equilibrate the system by simulating for time t_{eq} using timestep Δt (provided below). For efficient equilibration, rescale the velocities of atoms to the desired temperature T every 10 steps. Compute, write, and monitor the time-evolution of the total energy $E = (K+U)$ during equilibration. Implement functionalities to write output at low frequency ($\sim$10-20 times during equilibration) for atom coordinates, velocities, as well as system energies and temperature, all in separate files.

At the end of equilibration, switch off the velocity rescaling, and perform a *production* run for time t_{prod} (provided below). Save and retain the output data for future analyses.

e) Plot the time evolution of the potential energy, U, the kinetic energy, K, and the total energy, $E = K+U$, during the production run. Is the total energy conserved? Calculate and report the mean, the standard deviation, and the variance of E, U, and K. Calculate, plot, and report the time evolution of $\sum_i v_{x,i}^2$, $\sum_i v_{y,i}^2$, and $\sum_i v_{z,i}^2$, where $v_{x,i}$, $v_{y,i}$, and $v_{z,i}$ are the components of the velocity vector of atom i along x, y, and z direction, respectively, as well as their mean, their standard deviation, and their variance. Conclude on the principle of equipartition of the energy. Repeat the same simulation and analysis, but now with a time step, Δt, increased/decreased by one order of magnitude. Conclude on the stability of your implementation as a function of the magnitude of the time step, and explain the possible reasons for obtaining a chaotic behavior.

f) Using the same procedure as in (a-d), but now with $n \in \{6, 8, 10\}$ while keeping the number density constant, $\rho = 0.1\sigma^{-3}$, run simulations for 4000 time steps (2000 for equilibration and 2000 for production) to report on the efficiency of your MD engine scales with the number of atoms. Plot the average computing time (real human time) per time step, $t_{\Delta t}$, as a function of the the number of atoms, N. To obtain the scaling, fit a functional form, $t_{\Delta t} \sim N^{\alpha}$. What is the magnitude of α? Estimate the number of years it would take to complete your simulation with $n = 50$.

g) Using the trajectory obtained in (f) with $n = 10$, plot the velocity distribution resulting form the production run as a probability function $P(v^2)$. Compare your result with the analytical form of the Maxwell Boltzmann velocity distribution.

h) Using the same procedure as in (a-d), but now with $n = 6$ while keeping the number density constant, $\rho = 0.1\sigma^{-3}$, and with $r_{cut} \in 2.5\sigma, 3.25\sigma, 4.0\sigma$, run simulation for 4000 time steps (2000 for equilibration and 2000 for production). Perform the same analysis as in (e), and conclude on the stability of your implementation.

i) Write a short note on the conversion of real units to natural units. Specifically detail the conversions for length, time, energy, temperature and pressure. Enumerate, and provide the values of the quantities given in the table at the end of the exercise sheet in the natural units.

Numerical values of quantities to be used:

quantity	value (units)
k_B	1.38×10^{-23} (m^2 kg s^{-2} K^{-1}
ϵ	0.5 k_BT
σ	2.55×10^{-10} (m)
T	300 (K)
m	105.52×10^{-27} (kg)
Δt	10^{-15} (s)
t_{eq}	2000 Δt
t_{prod}	2000 Δt