Universität Freiburg – Institut für Physik
Applied Theoretical Physics
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Exercise 2 for '*Computational Physics - Material Science*', SoSe 2025
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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 codes should be commented, and the equations given in the pdf file have to be referenced in the source codes.

Exercise 2.1: LJ fluid-1: microcanonical ensemble in 2D

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 in 2D that computes the trajectory of a collection of N atoms interacting through the LJ potential in the microcanonical (NAE) ensemble, where A is the box area and E the total system energy.

Unless specified otherwise, values for the various quantities defined in *real* units at the end of the exercise sheet should be used. In our *real* units system, distance, energy, temperature, mass, and time are given in nanometers (nm), kilocalories per mole (kcal/mol), kelvin (K), grams per mole (g/mol), and femtoseconds (fs), respectively.

a) Consider a 2D square simulation box with dimension L along each direction containing $N = n^2$ atoms. The square simulation box is the region of space bounded by $[0 \leq x < L; 0 \leq y < L]$, and the atoms are initially distributed on a square lattice with a lattice parameter, a_{lat}, bounded by the simulation box. Implement such a geometry with $n = 20$ and a number density $\rho = N/A = N/L^2 = 0.25\sigma^{-2}$. Provide a snapshot of the initial geometry. (*hint:* *While developing your code, it is suggested to consider* $n = 5$.)

b) Assign randomly the initial component velocities (v^i_{x0}, v^i_{y0}) to each atom i, such that the initial temperature of the system is T_0 (provided below).
Hint:
   - *Assign initial component velocities randomly in the range* (-1,1).
   - *Shift all velocities by the mean to cancel the linear momentum of the system (you should have*

$$\sum_{i=1}^{N} v^i_{x0} = \sum_{i=1}^{N} v^i_{y0} = 0$$

   after the shift).

- *Rescale the velocities to achieve the desired temperature T_0.*

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 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 PBCs along each dimension and the Velocity-Verlet time integration scheme, equilibrate the system by simulating for time t_{eq} using a timestep Δt (provided below). For efficient equilibration, rescale the velocities of atoms to the desired temperature T_0 every 10 steps. Implement functionalities to write output with a desired frequency for atom coordinates, velocities, as well as system energies and temperature, all in separate files.(*hint: Refer to Sheet 01 for the output format of the trajectory data compatible with the Ovito visualization software.*)

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

e) Plot the time evolution of the potential energy, $\hat{U}$, the kinetic energy, $\hat{K}$, and the total energy, $\hat{E} = \hat{K} + \hat{U}$, during the production run. Is the total energy conserved? Calculate and report the mean, the standard deviation, and the variance of $\bar{E}$, $\bar{U}$, and $\bar{K}$. Calculate and plot the time evolution of $\sum_i v_{x,i}^2$, and $\sum_i v_{y,i}^2$, where $v_{x,i}$ and $v_{y,i}$ are the components of the velocity vector of atom i along x, and y, respectively. For each component, also compute and report the mean, standard deviation, and variance. Conclude on the principle of the equipartition of the energy, which states that in thermal equilibrium, each degree of freedom (e.g., velocity component) should contribute equally to the total kinetic energy. Repeat the same simulation and analysis, but now with a time step, Δt, (i) increased, and (ii) decreased by one order of magnitude. Conclude on the stability of your implementation depending on the magnitude of the time step.

f) Using the same procedure as in (a-d), but now with $n \in \{10, 20, 30, 40, 50\}$ while keeping the number density constant, $\rho = 0.25\sigma^{-2}$, run simulations for 100 time steps to report the scaling of the efficiency of your MD engine as a function of the number of atoms. Plot the average computing time (real human time) per time step, $t_{\Delta t}$, as a function of 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 $n = 1000$. Discuss a solution to improve the performance of your implementation for large n (*hint: implicit parallelization can be obtained by replacing 'range' by 'prange' in a loop, and using the numba decorator @njit(parallel=True)*).

g) Using the trajectory obtained in (f) with $n = 20$, plot the velocity distribution resulting from the production run as a probability function $P(v^2)$ where $v^2 = v_x^2 + v_y^2$ is the squared magnitude of the 2D velocity vector of a particle. Compare your result with the analytical form of the Maxwell Boltzmann velocity distribution.

h) With fixed $n = 20$ and keeping the number density constant, $\rho = 0.25\sigma^{-2}$, now vary the cut-off radius as $r_{cut} \in 3.25\sigma, 4.0\sigma$, and run simulations for 20000 time steps (10000 for equilibration and 10000 for production). Plot the time evolution of the potential energy, $\hat{U}$, the kinetic energy, $\hat{K}$, and the total energy, $\hat{E} = \hat{K} + \hat{U}$, during the production run, and conclude on the stability of your implementation.

i) With fixed $n = 20$, $\rho = 0.25\sigma^{-2}$ and $r_{cut} = 2.5\sigma$, run simulation for 20000 time steps (10000 for equilibration and 10000 for production) for $\epsilon \in \{0.1k_BT_0,\ 0.5k_BT_0,\ 1k_BT_0,\ 5k_BT_0\}$ (here T_0 is the desired temperature of the system). What do you observe when ϵ is increased from $0.1k_BT_0$ to $5k_BT_0$? To visualize this, for each value of ϵ, provide a representative snapshot (using Ovito) obtained during the production run.

Numerical values of quantities representative of Argon:

quantity	value (units)
k_B	0.0019849421 (kcal/mol/K)
ϵ	0.297741315 (kcal/mol)
σ	0.188 (nm)
T_0	300 (K)
m	39.95 (g/mol)
Δt	1 (fs)
t_{eq}	10000 Δt
t_{prod}	20000 Δt