CBE / MME 4428 INTRO TO NANOENGINEERING

Project: Molecular Simulation

Due: 3:30 pm, Thursday Nov. 30, 2023

Report Requirements

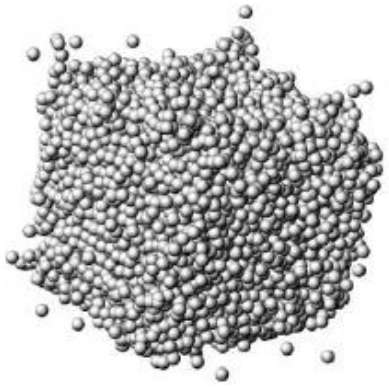
Submit a hard copy of your project report during class. In addition, submit to the OWL Drop Box tab any Excel, MATLAB, etc. files used to prepare plots or perform calculations. Equations need not be typed; legible hand calculations and sketches are acceptable.

The report must explain all calculations and present all numerical answers and requested plots. The grader will not search through Excel or other files to find plots or calculations.

Carry at least 6 significant digits in all calculations and present answers with at least 4 significant digits. Please take care to ensure that you arrive at the correct numerical answers and report the correct units. Include units and axes labels in all plots. Grading will be heavily weighted toward correct final answers.

You are encouraged to discuss the project with classmates, but sharing spreadsheets or codes is not allowed. Download the project data from your own OWL account as everyone has been assigned a different data set.

Late submissions will not be accepted.



Part 1:

The data provided in the "Part 1 Coordinates" and "Part 1 Parameters" sheets of "Project data.xls" in the Drop Box folder on OWL were generated from a molecular dynamics simulation performed at constant energy, volume, and number of atoms. The data table below summarizes the important parameters in the simulation, the values of which are given in the "Part 1 Parameters" sheet of "Project data.xls".

The simulation is of atoms of mass m that interact by a Stark-Müller potential, which is defined by,

$$V = \beta\left[\frac{1}{16}\left(\frac{\xi}{r}\right)^5 - e^{-r/\xi}\right]$$

where V is the potential energy of interaction between the pair of atoms, r is the distance between the atoms, and ξ and β are parameters that depend on the type of atoms.

The simulation imposes periodic boundary conditions on all sides of the simulation box, which extends from 0 to L in each direction. You are to ignore the periodic boundary conditions in force and energy calculations.

Description	Variable	Units
Index of main atom considered in calculations	M	–
Length of simulation box in each direction	L	Å
Timestep	Δt	s
Atomic mass	m	g/mol
Stark-Müller xi parameter	ξ	Å
Stark-Müller beta parameter	β	eV

The "Part 1 Coordinates" sheet gives the positions and velocities of all the atoms at a certain time. Note that atoms with coordinates listed as being outside of the 0 to L domain have crossed a periodic boundary without yet being moved back inside. Use the listed coordinate in force and energy calculations, but treat them as being inside the 0 to L boundaries for the density calculation.

a) Present a 2D plot of the (x, y) positions of all the atoms at this instant.

b) What is the density of the fluid (molecules/m^3)?

c) Calculate the total instantaneous kinetic energy (J) of the system.

d) Based on this instantaneous kinetic energy, what is the instantaneous temperature (K) of the system?

e) Using the ξ and β parameters that you have been assigned, plot the Stark-Müller potential energy as a function of distance between the atoms. Ensure that you select the axis limits to illustrate important features of the function.

f) Using a Lennard-Jones cut-off radius of 15 Å, calculate the total potential energy (J) in interactions between atom M and all other atoms.

g) Again using the snapshot data in the "Part 1 Coordinates" sheet and a cut-off radius of 15 Å, calculate the total potential energy of the system at this instant, ignoring the periodic boundary conditions.

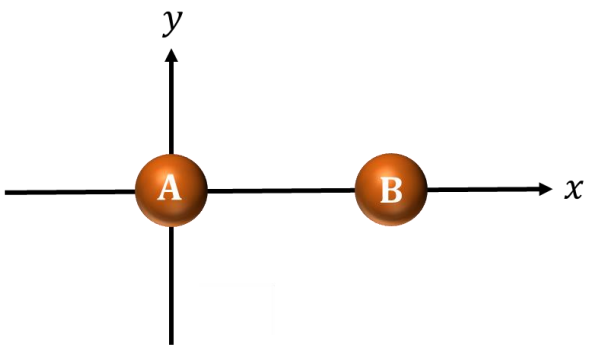
h) Derive an expression for the Stark-Müller force exerted by one atom on another.

i) What is the force (N) vector on atom M at this instant, again, using a cut-off radius of 15 Å?

j) Using a timestep of Δt in a modified Verlet scheme, calculate the position (m) and velocity (m/s) of atom M one timestep in the future. (For this part, assume that the velocity data in the "Part 1 Coordinates" sheet are actually one half timestep *behind* the position data. Calculate the new velocity and position one timestep in the future, though still offset one half timestep from one another).

Part 2:

In this part, you will perform a Metropolis Monte Carlo simulation to calculate the average potential energy between two atoms interacting by a Lennard-Jones potential and constrained to the x-axis. The atoms are at equilibrium with a reservoir at temperature T. The "Part 2" sheet of "Project data.xls" provides the σ and ε parameters of a Lennard-Jones potential and the temperature, T, that you will use in your simulation.



In your calculations, keep Atom A fixed at position $x = 0$ Å. Atom B can move along the positive and negative sides of the x-axis. Use a maximum step size of $\Delta x = \pm 0.5$ Å, start with the atoms 10 Å apart, and include 10,000 attempted moves in your calculation.

Suggested column headings for a possible Excel implementation of the simulation are provided below.

Complete the simulation.

Step	Properties of new microstate (attempted move)		Accept/reject decision			Properties of sampled microstate	
	Position of Atom B [Å]	Potential energy [J]	Probability of acceptance	Random number	Accept / reject?	Position of Atom B [Å]	Potential energy [J]
0	—	—	—	—	—	10	
1							

k) Using a 0.1 Å bin size, plot a histogram of the position of Atom B. Discuss the results.

m) Based on your simulation results, calculate the average distance (m) between the two atoms, $\langle x \rangle$.

n) Based on your simulation results, calculate the average potential energy (J) of interaction between the atoms, $\langle E \rangle$. Discuss the reliability of this calculation and how that can be assessed.

p) Compare your calculated average potential energy to the predictions of equipartition theorem and discuss the results.

q) If the system temperature were slowly lowered to 0 K, what would be the average potential energy (J) of interaction between the atoms, $\langle E \rangle$, and average distance (m) between the two atoms, $\langle x \rangle$?