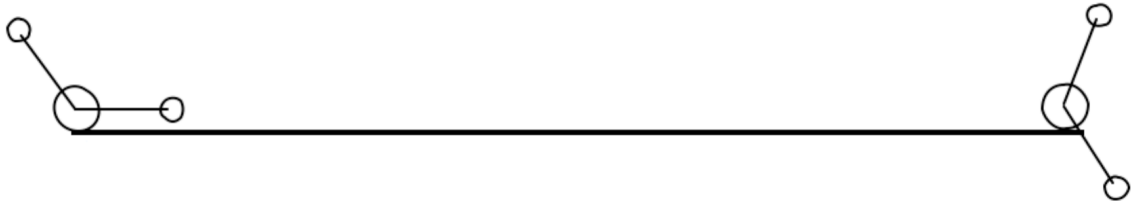


CE 530
Molecular Simulation

Assignment #7

Due: 18 April 2017

1. The SPC (Simple Point Charge) model for water is very popular. It consists of a single Lennard-Jones site, representing the oxygen atom, and three partial charges to describe the hydrogen atoms and the molecule's electrostatic features. The LJ size parameter (σ) has the value 3.166 Angstroms, and the energy parameter (ϵ/k_B) is 78.23 K. The charge on each hydrogen atom is $0.41e$, where e is the charge of an electron; the charge on the oxygen is $-0.82e$. The oxygen-hydrogen distance is 1.0 Angstrom, and the HOH bond angle is 109.5 degrees.
 - a. Compute the dipole moment for this model. Report your answer in Debye.
 - b. Consider two such water molecules oriented such that they each lie in the x-z plane, with one of the OH bonds coinciding with the x-axis; see figure below (not to scale). Their OO separation is 9 Angstroms. Compute the interaction energy of the pair. Report your results in two ways: first in units of the LJ energy parameter (ϵ), and then in kJ/mole (obtain the value per mole by multiplying by Avogadro's number).



- c. Repeat part (b), except omit interactions of one molecule with both hydrogens of the other. That is, consider that one molecule lies at the origin, and the other is at the edge of a 9-Angstrom cutoff, such that the O atom is inside the cutoff but the H atoms are not. Report your answer in the units requested in (b).

2. The file [config.dat](#) contains the xyz coordinates from one configuration of a simulation of 6000 Lennard-Jones atoms in a cubic box of edge length 20σ (where σ is the Lennard-Jones size parameter) ([image here](#)). Each row of the file gives x, y, and z coordinates (3 values) for one of the atoms.

For this problem you are to compute the radial distribution function $g(r)$ for this configuration. Submit the following to complete the assignment:

- (a) A plot of the function $g(r)$. You can do this in Excel (or your preferred graphing package) using the output of your calculation.
- (b) The source code used to generate $g(r)$ from the data.

You may use any programming language or application that you're most comfortable with to do this (I suggest you do not attempt to do this problem by hand, even if you're good at arithmetic, using a calculator, and have nice graph paper). A Java class is available [here](#) with code included to read and write data, if you wish to use that; if you do, then you need to write just the missing part of the method that does the $g(r)$ calculation. Remember to use the minimum image when you compute the separation between two atoms.

config.dat: <http://www.eng.buffalo.edu/~kofke/ce530/Assignments/config.dat>

image: <http://www.eng.buffalo.edu/~kofke/ce530/Assignments/config.png>

Java file: <http://www.eng.buffalo.edu/~kofke/ce530/Assignments/Assignment7.java>