Modeling Benzene in a Vacuum

PHY494: Final Project Proposal

Nikolaus Awtrey, Justin Gens, Ricky Sexton

1 Problem

We are going to start by modeling a single benzene molecule–using a purely classical approach– to find the parameters that produce experimentally determined properties of benzene. Once the model has been built, more benzene molecules will be added to the system and classical MD will be performed. Benzene (C_6H_6) has an inner ring of carbon atoms where the bonds alternate between single and double bonds, and each carbon atom has a single-bonded hydrogen atom. This gives rise to several different bonded (C-C single, C-C double, H-C single) and non-bonded (C-C and H-C) interactions within the molecule itself. For bonded interactions, pairs of atoms will be modeled via The Morse potential

$$V_M(r) = D_e\big(1 - e^{-\beta(r-r_e)}\big)^2. \tag{1}$$

The non-bonded interactions will be modeled via the Lennard-Jones potential

$$V_{LJ}(r_{ij}) = 4\big[(r^*_{ij})^{-12} - (r^*_{ij})^{-6}\big], \qquad r_{ij} = \sqrt{(\mathbf{x}_j - \mathbf{x}_i)^2}. \tag{2}$$

Our problem is particularly interesting because most of the interactions in benzene are non-classical phenomena. If this problem were solved *properly*, every electron in each atom would have to be accounted for; however, this gets complicated quickly and may be impossible to model computationally. Thus, our goal is to find the properties of benzene that can be reproduced in a classical model.

2 Approach

Our first step is to find units which will minimize the error associated with running the calculations. Then, we will make a file to compile all initial data (i.e. positions, masses, type, etc.) for each atom in the structure using the accepted values. Once we have our initial data, we will use the harmonic oscillator potential to write the function that calculates the forces between pairs of atoms. This force function will be integrated (using the RK4 algorithm) over to produce a trajectory for all particles. Initially, it will be floppy since there will not be an applied torque keeping the molecule mostly planar. The next, and most difficult step, will be to create a new function that holds the atoms roughly in the desired region, and determine parameters which produce accepted properties of benzene.

3 Objectives

- Create array of all positions of atoms
- Assign random velocities based on initial temperature
- Develop a total force function that can be integrated over a short time period
- Find parameters for the initial positions and spring constants that produce a stable molecule
- Implement additional restoring force that creates a stable improper dihedral structure
- Find parameters that produce a stable, fairly rigid simulation of a benzene molecule
- Simulate interactions of multiple benzene molecules
- Deduce heat capacity of benzene from system of molecules