Modeling Benzene in a Vacuum

PHY494: Final Project Proposal

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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. For this project we have decided to use Lennard-Jones units, since it is a very convenient way to work with the LJ potential, masses in general, and system momentum. Next, we will write code that generates the initial positions of all atoms in a benzene molecule. This will be designed to be scalable such that we can later go back and generate N benzene atoms and see how they interact with each other as a system. Once we have our initial positions, we will use the potentials above to write a function that calculates the forces between pairs of atoms. This force function will be integrated 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

1. Develop an MD code that solves Newton's equations of motion for a molecule in a vacuum
2. Generate initial conditions of benzene molecules based on online resources
3. Develop an algorithm that outputs initial positions of all atoms for a single benzene molecule, and assign random velocities (in a specific range) to all atoms in molecule based on initial temperature

4. Develop a total force function that can be integrated over a short time period using velocity Verlet and RK4 algorithms
5. Compile a list of parameters from various existing force-fields for the initial positions and spring constants that produce a stable molecule
6. Implement additional restoring force that creates a stable improper dihedral structure
7. Find parameters that produce a stable, fairly rigid simulation of a benzene molecule

4 Stretch Objectives

1. Simulate interactions of multiple benzene molecules
2. Deduce heat capacity of benzene from system of molecules