Activity 2A: MD simulations of alkanes

Overview

In this exercise we use the OpenMM application/library to carry out a common MD simulation protocol to generate trajectories of two simple hydrocarbons in the gas phase: ethane and butane.

Basic simulation protocol

Most research-grade MD simulations follow the same basic protocol:

1. A brief energy minimization to eliminate “bad” interatomic contacts (i.e., ones that would cause high forces) that would result in a numerically unstable simulation.
2. A relatively brief MD simulation for the purpose of bringing the system temperature (NVT) or temperature and volume (NPT) to the desired equilibrium values.
3. A long MD simulation (often deemed “production”) for the purpose of collecting data.

We will implement a similar protocol using OpenMM to study the gas phase behavior of ethane and butane.

Worked application: ethane

The notebook *ethane_BasicMD_OpenMM.ipynb* contains all of the necessary commands to use OpenMM to carry out a gas phase simulation of a single ethane molecule. As written, it requires the files *ethane.gaff2.xml* (force field information) and *ethane.pdb* (starting coordinates and topology) to be in the same directory as the notebook.

Briefly, this notebook will carry out:

1. Up to 100 steps of energy minimization using the L-BFGS algorithm.
2. A 5.0 ps MD simulation to bring the ethane molecule to an equilibrium temperature of 298 K (25 °C) in which output is printed every 0.2 ps (100 steps).
3. A 20 ns MD simulation at 298 K in which output is printed every 500 ps and structures are saved every 0.2 ps into a file called *ethane_sim.dcd*. (This trajectory file is written in a commonly used binary format called DCD.)

Download and run the notebook. These simulations take about 1.5 minutes to complete on a 2012 MacBook Air. (Your mileage may vary!)

Your turn: butane

Create a copy of the ethane simulation notebook called *butane_BasicMD_OpenMM.ipynb*. [Creative name, right?] Modify this notebook to:

1. Read in the files *butane.gaff2.xml* and *butane.pdb*.
2. Carry out a 10 ps MD simulation to bring the butane molecule to an equilibrium temperature of 298 K in which output is printed every 0.5 ps. [Leave the minimization portion beforehand unchanged.]
3. Carry out a 40 ns MD simulation at 298 K in which output is printed every 1 ns and structures are (still) saved every 0.2 ps into a file called *butane_sim.dcd*.

After you've made these modifications, go ahead and run the notebook. These simulations take about 6 minutes to complete on a 2012 MacBook Air. We will discuss some of the nuances to these simulations (and the previous ones) as they run.