Activity 2B: Trajectory analysis of alkane simulations

Overview

In this exercise we will use the MDTraj library to carry out analyses of the MD simulation trajectories that we've produced for ethane and butane. We'll also use the NGLview library to visualize the trajectories themselves.

A quick reminder/introduction

In the previous exercise we generated trajectories (i.e., a time series of atomic coordinates) for two small molecules. The goal of trajectory analysis is to extract *useful* (i.e., to a human) information from these time series. For these molecules we'll look at bond lengths, angles, and torsion angles.

Worked application: ethane

The notebook *ethane_TrajectoryAnalysis_MDTraj.ipynb* contains all of the necessary commands to use MDTraj to carry out an analysis of your ethane simulation. As written, it requires the files *ethane.pdb* (topology) and *ethane_sim.dcd* (trajectory) to be in the same directory as the notebook.

Briefly, this notebook will carry out analyses of:

1. The H-C-C-H torsion angle, specifically defined by the atoms H11-C1-C2-H21. [This specific choice of atoms doesn't really matter, as the resulting data would be identical for any atoms H1X-C1-C2-H2Y, where X,Y={1,2,3}. Why?]
2. The C-C bond length.

In both cases we will first construct a histogram of the observable and then convert the histogram counts into a potential of mean force (pmf) that will recast the count data/probabilities as relative free energies.

Download and run the notebook. The analyses should run very quickly.

Your turn: butane

Create a copy of the ethane analysis notebook called *butane_TrajectoryAnalysis_MDTraj.ipynb*. Modify this notebook to:

1. Read in the files *butane.pdb* and *butane_sim.dcd*.
2. Analyze the C-C-C-C torsion angle. [There's only one unique atom selection possible.]
3. Analyze the C-C-C bond angle. [Use either C1-C2-C3 or C2-C3-C4.]
4. Make only a histogram of one of the C-H bond lengths. [Pick any bonded C-H pair, CX-HXY.] What do you notice about the distribution of this bond length? [What's going on here?]

Optional activity for those seeking more thrills:

Increase the value for `integrator.setConstraintTolerance` by a couple of orders of magnitude and re-run your butane simulation. Then see how the C-H bond length distribution changes!