**Activity: 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.

**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 (only one unique atom selection).
3. Analyze the C-C-C bond angle (use either C1-C2-C3 or C2-C3-C4).
4. Analyze 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?)