Homework Assignment 4 – System Energy Calculation

DUE Thursday, Oct 5.

Fetch the file */home/compbio/Shared/Hmwk4.pdb* from kirin.kit.jhu.edu to a new directory under your permanent home directory on a Mac. Write a python program to read in the system coordinates in this Argon configuration file and calculate the **potential** energy (in SI units) of the system with the functions and parameters used in your MC simulation.

The program should assume periodic boundary conditions and print out the answer in labeled format with appropriate units. **The program should run as a standalone script** – it should not need *mc_params* or *modules.py*, i.e. you should copy and paste the necessary functions from *modules.py* into your program. Email a working version of your program to Dr. Fleming (pat.fleming@jhu.edu). The program must run as-is for credit.

Hints:

- Everything you need is in the *mc_nvt.py* and *modules.py* files.
- Instead of reading in *mc_params*, make the dictionary inside your script as shown in lab1d, but use the values in the *mc_params* file.
- You can copy and paste any of the functions in *modules.py* into your script and then you don't have to import them – just call them directly (put them near the top of your script).
- Test your program after every edit.
- **Do not do a simulation**; just print out the total energy of the system.
- Points will be taken off for inclusion of unnecessary code lines (e.g. import something only if you need it; define something only if you use it).
- Although you could start with *mc_nvt.py* and just comment out lines, in view of the rubric just above, it may be better to copy and paste the necessary code from *mc_nvt.py* into your new script along with the necessary functions from *modules.py*.