This computational exercise again builds on computational exercise #4. But this time, you will calculate the mean bond length for the HF bond (a) as an average over the spline fitted energy function, (b) using a Langevin dynamics simulation and (c) using the Metropolis algorithm for Monte Carlo. I (Prof. Snyder) do not have a separate worksheet for this exercise (we'll cover the relevant theory in lecture on Friday mid-day). Rather just fill in the code as indicated in the attached Jupyter notebook, run your code for two different temperatures: 0.00094 (room temperature, in atomic units) and another temperature of your choosing and answer the following questions:

(1) At room temperature, which method, the "time" average for the Langevin simulation or the Monte Carlo calculation, produced a more "accurate" (i.e. closest to your average bond length as calculated as an average over the spline fitted energy landscape) result? At your other choice of temperature, which method produced the more "accurate" result?

(2) How accurate were the bond lengths calculated as compared with the experimental value of 0.917 Angstroms (ref:  <https://cccbdb.nist.gov/exp2x.asp?casno=7664393&charge=0#NISTdiatomic>, although I am not sure at what temperature the experiment determining this value was performed)?

(3) How did temperature affect the average bond length, if at all?

1.) The Monte Carlo calculations had a more accurate result for T = 0.00094. The Monte Carlo calculation was more accurate for T = 0.002.

2.) the bond lengths were fairly accurate using T = 0.00094. r average had a 0.2% error mean bond length had a 0.7% error and Monte Carlo had an error of 0.1%. increasing the temperature looks to increase the error but not by a lot.

3.) The bond length increased in length when temperature was increased from 0.00094 to 0.002