Computational Lab#6 – HF Average bond length calculations 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?

**Langevin’s calculation was closer to the avg. bond length. At room temp., even when I increased the temperature, it was still closer.**

(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)?

**The bond lengths were pretty accurate and very close to the experimental bond length.**

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

**As the temperature increased, the bond length decreased and the opposite is true for a decrease in temperature.**