Problem Set # 2

Due @ 11:59 pm Thursday 2/28 by electronic submission on BlackBoard

1. *N*-butanol ($CH_3CH_2CH_2CH_2OH$) occurs naturally as a minor product of fermentations. You are asked to enumerate all possible conformers for the isolated *n*-butanol molecule in the gas phase, using the MM+ force field. In your solution, please make sure to provide a schematic indicating which torsional angles you have varied, and a table listing the values of these angles for the various conformers.

2. Using the results of Problem 1, compute the mean distance between the oxygen atom and the carbon atom at the opposite end of the *n*-butanol molecule (a) at 0 K and (b) at 300 K.

3. (a) Compute the average and standard deviation of each of 20 sets of 50 uniformly distributed random numbers between 0 and 1 (i.e., 1000 random numbers in total). Report the 20 set averages (or "means") and standard deviations in a table, but do not report the individual random numbers. You may use Excel, Matlab, or any other environment you prefer to generate these data.

   (b) Obtain a theoretical estimate of the expected standard deviation of the 50-number samples and compare it to your observations in (a).

   (c) What is the distribution followed by the mean values of the 20 sets? Can you estimate theoretically the probability of observing a set with a mean less than 0.45? How do your measurements compare to this expectation?

4. Generate the Cartesian coordinates (x,y,z) for 500 uniformly distributed points on the surface of a sphere of radius 1. Explain in detail how you obtained these points., but report only a small sample of 10 points. Plot the distribution of z values for the 500 points; what theoretical distribution do you expect these points to follow? Is this expectation confirmed by your actual data?

5. We would like to generate a set of random values with probabilities proportional to $x \exp(x)$, for x between 1 and 2. Propose an algorithm to do so. Confirm that your proposed algorithm works by generating 200 such points and comparing their distribution to the desired functional form. Show a "histogram" plot of your 200 points superimposed over the theoretical distribution.

Please submit your results and graphs electronically, as a single PDF file. Also submit any codes (e.g., Matlab scripts, or Excel worksheet files), properly labeled and commented. We will assign 20% of the grade to the "aesthetics" of your solution: how easy it is to follow, quality and proper labeling of graphs and column headings, commenting of codes, etc.