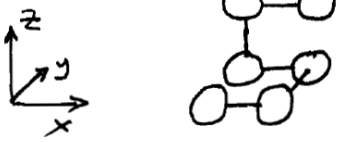
Assignment 5 – Due Dec. 15th by electronic submission to azp@princeton.edu

Pick ONE of the two problems below.

Problem 1

Consider a simple cubic lattice polymer model (in 3 dimensions). Each bead of the chain occupies a single lattice position. Two beads cannot occupy the same position ("excluded volume" interaction). The energy of non-bonded neighboring beads is –1 in reduced units. For example, the hexamer (r=6) configuration shown to the right has energy equal to -2 units.



a) A simple algorithm to generate random configurations of the chain is the following: Starting at one end, proceed along a random direction. Check to see if the excluded volume condition is satisfied. Stop when you have reached the desired chain length. Using this algorithm, calculate the mean end-to-end distance, $\langle R_e \rangle$ (R_e = distance from first to last bead) and mean energy $\langle U \rangle$ at inverse temperatures, β=0, 0.3 and 1 for r =4 and r=20, along with their statistical uncertainties. Also report the fraction of successful chain growth attempts, f.
b) Implement the Rosenbluth algorithm for this system and obtain $\langle R_e \rangle$, $\langle U \rangle$ and f for the same conditions as above.
c) Use the Rosenbluth algorithm to find the scaling exponent ν of the end-to-end distance with chain length, $\langle R_e \rangle \propto r^{\nu}$ for β=0, 0.3 and 1. How do your exponent values match the values discussed in class?

Problem 2

Modify an NVT Monte Carlo program for the LJ fluid (yours, mine or Frenkel and Smit's) so that it now performs Wang-Landau sampling instead of Metropolis sampling.

d) Obtain the entropy (density of states) for a LJ system with L=5, N=110 for energies between -700 and -500.
e) Investigate the effects of changing the cutoff value for the modification factor g and the "flatness" criterion on the calculated density of states.
f) Repeat the calculation for energies from -800 to -650. Do your two densities of states agree in the region of overlap?

Please submit your solution (graphs, comments, code lines that you added) as a single PDF file. I will assign 20% of the grade to "aesthetics" of your solution: how easy it is to follow, quality and proper labeling of graphs etc.