Lab-17

1. Consider the 1 D Ising model Hamiltonian H = -J $\sum_{<ij>} S_i S_j - h \sum_i S_i$(you can take J to be 1, whcih basically means we will be measuring all energies in the problem in units of J), where $\{S_i\}$ are set of N spins that can take $\pm$ 1 values. Set up a Monte-Carlo simulation using Metropolis algorithm to study the thermodynamics of this system and find the variation of the following quantities with temperature/field:

   Magnetization, $m = \frac{1}{N} < \sum_i S_i > Vs. k_B T$ (for h = 0, 1)
   Energy per particle $u = \frac{<E>}{N} Vs. k_B T$ (for h = 0, 1)
   m Vs. h for $k_B T = 1, 0.$
   $Specificheat$,$c_v \frac{}{k_B}$ Vs. $k_B T$ (for h = 0). Note that $\frac{c_v}{k_B} = \frac{1}{N^2}(< E^2 > - < E >^2)\beta^2$

   Few points to keep in mind:

   It is usual to use what is known as periodic boundary conditions which means the last spin has the first spin to its right and consequently the 1st spin has the last spin to its left. This cuts down any boundary effects that might plague your simulation when the system size is small. Going over the entire set of spins once (flipping and accepting or rejecting states using Metropolis rule) is called a single MonteCarlo sweep. You can average using state after each MC sweep. The number of sweeps should be large. You may start off always with the aligned state (all spins pointing in one direction). At high temperatures this will get randomised in no time and at low temperatures this will allow for fast equilibriation. In any case, you will need to reject the first set of MC sweeps (10000 or so to be safe) as you may not have hit the steady state.