Chemical Engineering I5800 Molecular Simulation Spring 2019

Problem Set 1 – due Feb. 14 or 21

1. (a) Using Monte Carlo numerical integration, find the volume inside an n-dimensional unit sphere for $n = 2, 3, 4$ and 5, and show that the result converges to the exact answer as 1/(number of tries) for all n.

   (b) Use importance sampling and Monte Carlo integration to compute

   $$\int_0^1 dx \, \frac{e^{-10x}}{1+x}$$

2. (1-d Ising model) Consider a one-dimensional periodic lattice with N sites, each of which has a "spin" which can be up or down, $s_i = \pm 1$. Each spin interacts with its neighbors to each side with an energy which favors alignment of the spins – negative when both are up or both are down, and positive otherwise. The explicit form of the total energy is

   $$E = -\epsilon \sum_{i=1}^{N} s_i s_{i+1}$$

   and the periodicity is taken into account by identifying $s_{N+1} = s_1$.

   Compute the average energy and the average spin of the lattice as a function of temperature using Monte Carlo simulation. To do this, pick a site i at random or else sweep though the lattice, change $s_i \to -s_i$, and accept or reject the change by the Metropolis rule. Do this for $N = 100$ at temperatures $k_B T = \epsilon/2$ and 2ϵ. In each case, run the simulation until the average energy stabilizes.

Random number generators and the code for the simple 1-d example of Metropolis Monte Carlo coding discussed in class (baby_mc.f) can be found on the course Backboard page.