CE 530
Molecular Simulation

Assignment #5 Due: 14 March 2017

1. Repeat problem 1 of Assignment 4, in which you computed the integral of a simple function using importance sampling Monte Carlo. However, instead of generating the points from a transformation of a uniform deviate, apply a Markov chain to produce points with the same limiting distribution.

2. Program a molecular simulation of an ideal gas in the isothermal-isobaric or grand-canonical ensembles, and run it to collect data that demonstrates the ideal-gas law (either pressure or chemical potential versus density). Plot your data (with confidence limits) and compare to the expected ideal-gas behavior.

   Since the molecule coordinates are not relevant to the behavior (the energy is always zero), your simulation needs to sample only the volume V or the number of atoms N (depending on which ensemble you choose), so this is much simpler than programming a full simulation. You don't have to move atoms around or worry about periodic boundaries, etc. In fact, you don't have to code atoms in at all; you need just a count of how many are there. You will encounter a number of minor details to think through, but it shouldn't take very much coding to get a working simulation.