Computational Physics Homework Set #5

(Due 12/17, at noon)

1) Consider the Ising model in a square lattice in two dimensions of size $L = 50$ with free boundary conditions. Normalize the maximum magnetization to unity (i.e. all spins up).

a) Use the Metropolis algorithm to find the equilibrium state at a given temperature, choosing the number of Monte Carlo steps per spin $t_n = n/L^2$ such that a "cold" initial condition (e.g. all spins up) and a "hot" initial condition (all spins random) gives approximately the same magnetization after n flip proposals.

b) Calculate the magnetization as a function of temperature and make a plot of it, comparing with the analytic prediction of the critical temperature $k_B T_c = 2.269J$. At each temperature calculate the magnetization by averaging over 5 seeds of initial "hot" conditions, each of them evolved through t_n steps of the chain.

2) Consider thermal equilibrium for a gas of N particles of equal mass m in 1 dimension under gravity ($N = 200$). Neglecting interactions between particles, write the potential energy as $U = \sum_{1=1}^{N} \phi(x_i)$, with the potential being $\phi(x) = mgx$ for $x > 0$ and $\phi(x) = \infty$ for $x < 0$ (that is, there is an impenetrable wall at $x = 0$).

a) You may choose units so that $m = g = 1$ and temperature such that $kT = 1/2$. Start from initial conditions where e.g. all particles are at the same location $x \equiv 1$.

b) In your Metropolis algorithm you should choose ϵ so that proposals for moving the particles $x_i^{(n+1)} = x_i^{(n)} + \delta x$, where $x_i^{(n)}$ is the position of particle i at step n, are roughly accepted half of the time. Here δx is a random variable uniform over the interval $(-\epsilon, \epsilon)$. *Explain* how you arrived at the ϵ value you took.

c) Run your Metropolis algorithm and compute and plot the potential energy as a function of Monte Carlo step number. From this plot, estimate the *equilibration time* of your Monte Carlo chain.

d) Using only data from your chain after the equilibration time, compute the average potential energy. Compare your value to the expected value in a Botzmann distribution, $\langle U \rangle = N \int mgx\, \mathrm{e}^{-mgx/kT} dx / \int \mathrm{e}^{-mgx/kT} = NkT$. Using the same data, compute the *rms* fluctuations about $\langle U \rangle$, that is $(\delta U)^2 = \sum_{\text{chain}} (U_n - \langle U \rangle)^2 / N_{\text{chain}}$,where N_{chain} is the number of steps in your chain after equilibration.

e) Compute the correlation function of the potential energy, $C(m) \equiv \sum_{\text{chain}}(U_n - \langle U\rangle)(U_{n+m} - \langle U\rangle)/(\delta U)^2$. Note that $C(0) \equiv 1$. Plot $C(m)$ as a function of step separation m and from this estimate the *correlation time* of your chain.

f) Using now only chain data after equilibration time that are *separated from each other by the correlation time* compute a histogram of particle positions. Compare this with the expected Boltzmann distribution per unit length $f(x) = mg/(kT)\,\mathrm{e}^{-mgx/kT}$.