PC5215, Numerical Recipes with Applications, Lab 3
(due Thursday, 26 Oct 2017)

1. The honeycomb lattice due to graphene by now is very famous. In this lab, we simulate an Ising model on a finite piece of a honeycomb lattice using Monte Carlo method. At each site, there is a spin $\sigma=\pm 1$ connected to three nearest neighbors. We assume that the energy contribution from a single neighbor is given by $-J\sigma_i\sigma_j$ for the nearest neighbor site i and j. The total energy E is the sum over the neighbors. We choose the spin coupling constant $J = 1$ (also $k_B = 1$). Write a program to implement the single-spin-flip Metropolis algorithm for the Ising model on honeycomb lattice. Compute the specific heat c (heat capacity per site) according to the formula

$$c = \frac{1}{k_B T^2 N}\left(\langle E^2\rangle - \langle E\rangle^2\right),$$

where k_B is the Boltzmann constant, T is temperature, N is the total number of spins. Present a plot of c vs dimensionless temperature $k_B T/J$ for several system sizes (say about 100 to 1000 spins). Locate the critical temperature T_c approximately by the specific heat data, and compare with the known result (exact result of T_c does exist for this model).