College of Science and Engineering
School of Physics & Astronomy

Modelling and Visualisation in Physics

SCQF Level 10, PHYS10035

Tuesday 30th April 2013

14:30 - 17:30

Chairman of Examiners
Professor S Playfer

External Examiner
Professor D McMorrow

Answer all six questions overleaf.
Completed codes should be uploaded via Learn as a single zip file immediately after the examination has finished. Alternatively, you can email the zip file to dmarendu@ph.ed.ac.uk.
Figures should also be submitted electronically, they should also be described in the script book.
You may use any resources available on the internet at the beginning of the examination, or present in your CPlab home directory but you may not communicate with any other person electronically or otherwise.

The bracketed numbers give an indication of the value assigned to each portion of a question.

Only the supplied Electronic Calculators may be used during this examination.

Anonymity of the candidate will be maintained during the marking of this examination.

Consider a model of cells on the square lattice, defined by the following energy function:

$$E(\{\sigma_i\}) = -J \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j}$$

where $J > 0$, i and j denote positions on the lattice, σ_i can take any of the values 0, 1 or 2, while $\langle ij \rangle$ denotes that the sum is performed over cell pairs which are nearest neighbours on the lattice. Finally, δ is the Kronecker delta: $\delta_{i,j}$ =1 if $i = j$, and 0 otherwise.

According to the Boltzmann distribution, the probability of observing a given configuration $\{\sigma_i\}$ is given by

$$P(\{\sigma_i\}) = \exp\left[-E(\{\sigma_i\})/(k_B T)\right]$$

where k_B is the Boltzmann constant and T is the temperature.

This model is known as the "Potts model".

1. Describe how you expect the typical states of the system to be at high and low T. How many degenerate ground states are there in this system for $T \to 0$? Describe what these are. **[2]**

2. Write a Java program to sample via Monte Carlo the equilibrium states in the Potts model on an $L \times L$ two-dimensional square lattice, with periodic boundary conditions. Your program should provide some means to choose the dimension L, as well as the value of the temperature T. It should also display the state of the system in real time as it is running. You may for instance initialise the lattice randomly, such that each cell starts in either state 0, 1 or 2 with equal probability. To set up the Monte-Carlo algorithm, use an update rule which attempts to modify a single cell at a time. **[25]**

3. Here and in what follows, you should set $J = k_B = 1$, and you can set $L = 50$. Use your code to compute the values of the fraction of cells in state 0, 1 or 2 as a function of time (in Monte-Carlo sweeps) for a given choice of the random seed to set the initial condition, and $T = 0.5$. Plot a set of curves for a choice of the seed. Estimate the equilibration time in your runs. **[3]**

4. Use your code to compute the average energy, and the variance of the energy, defined as

$$\langle E^2 \rangle - \langle E \rangle^2,$$

for a range of temperatures (note that $\langle \cdot \rangle$ indicates an average). You should plot the average energy and the energy variance versus temperature, and in the latter plot you should include error bars. You can concentrate on T between 0.3 and 2.5. Your plot of the energy variance versus T should have a peak: why? What does the temperature at the peak correspond to? **[10]**

5. Modify your code so that before attempting to update a cell according to the Monte-Carlo algorithm you set up previously, you "mutate" a cell as

follows. With probability p, if the state of the cell is 0, you update it to 1; if the state is 1, you update it to 2; if the state is 2, you update it to 0. (The cells chosen for the mutation and the standard Monte-Carlo update need not be the same; the suggestion is that you choose both of them randomly). **[4]**

6. Compute the average energy and the energy variance as a function of T for $p = 0.03$. Plot, and comment, the resulting curves. In particular, say why you think the peak position has now shifted in the variance plot, with respect to the $p = 0$ case. You do not need to include error bars for any of these plots. **[6]**