PY 421 - Introduction to Computational Physics

Homework # 8. April 17, 2013.

Due on Friday April 26 at discussion time (3PM).

The assignment:

Subject of this assignment is the Potts model. You should modify a program, use it to perform Monte Carlo simulations collecting the data, derive the relation between specific heat and energy fluctuations, and graph the data you obtained.

Problem 1

Modify the code potts.f90 in the following manner.

The new code should open a file called `input` and should read from this file the parameters for the simulation. The code should also open a file called `output`.

The first line of `input` will contain 3 numbers, namely the value of q, the *saved_seed* and a *cold_hot* integer variable that will be 0 or 1 for a cold start or hot start, respectively.

The following lines will contain four numbers each, namely the value of *beta*, the number *ndisc* of measurements to be discarded, the number of measurements *nmeas* that must be made after the discarded measurements, the number *nit* of iterations per measurement (whether discarded or performed).

The code should get the parameters for starting the simulation from the first line. It should then set the value of *beta* according to the second line and perform a total of $(ndisc + nmeas) * nit$ Metropolis Monte Carlo iterations, collecting results over the *nmeas* measurements. The code should then read the next line, set the *beta* to the new value and perform the required number of Monte Carlo iterations **without resetting the seed or the values of the spins**, and so on, until all input lines are read. Thus, altogether the program will run just one long simulation during which the values of *beta* are changed according to the values in the `input` file.

At each measurement the code must measure two quantities:

1) The energy E per bond, defined as sum of all bond energies divided by the total number $2N^2$ of bonds.

2) The correlation m defined as follows: we consider pair of spins s and s' whose coordinates (both x and y) differ by $N/2$ and associate to this pair a number equal to 1 if $s = s'$, equal to $-1/(q-1)$ if $s \neq s'$. m is the sum of these numbers over all pairs, divided by the total number $N^2/2$ of pairs. Please notice that, because of the periodic boundary conditions, given a spin s there is only one spin whose coordinates differ by $N/2$ from those of s and that the total number of such pairs is $N^2/2$. m is defined in such a way that if the system is fully "magnetized", i.e. all the spins take the same value, $m = 1$, while if the spins half a distance apart along the diagonal (as far as we can go with periodic boundary conditions) are totally uncorrelated, then $m = 0$.

The code must accumulate these quantities as well as E^2 and, at the end of the *nmeas* measurements, it should write on a single line of `output` the values of *beta*, of the average energy per bond $< E >$ (averaged over the *nmeas* measurements), of the mean square fluctuation of E multiplied by the number of bonds $C = 2N^2(< E^2 > - < E >^2)$, and of the average (always over the *nmeas* measurements) of the correlation $< m >$. The code should write one such line for each of the values of *beta* in the `input` file.

You should remove from the current code potts.f90 the redundant measurements (of the acceptance and of the variable mag). **Remove also all print statements.**

For this problem, you should return your modified program.

Problem 2

You should run your modified program to perform four simulations of the Potts model. You will be assigned the value of q in a separate message. For that value of q you should perform two simulations on a system with $N = 32$ and two simulations on a system with $N = 64$ (I recommend that you leave the value of N as a parameter in the code, i.e. do not modify the code introducing allocatable arrays for the spins, but rather compile two times with the two different values of N and use the two separate executables). For each value of N the two simulations will be from a hot start and ascending *beta* and a cold start and descending *beta*. You will find the input files for all simulations in the ∼rebbi/courseware/code directory with obvious notation

(e.g. potts_input.q3n32c is for the simulation with $q = 3$ $N = 32$ and cold start). I have written the input files so as to explore the regions of the phase transition with somehow greater detail. **You should copy the `output` files of your simulations to files with the same extension as the input you used.** For example, if you used potts_input.q3n32c copy the output to output.q3n32c. Make sure to copy the output before you run another simulation, otherwise the output file will be overwritten. Allow some time for running the simulations.

For this problem you should return the output files of the four simulations.

The simulations with N=64 may run for several minutes. I recommend that you compile the code with the -O3 optimization flag to speed up execution, e.g., assuming that you are compiling the code with N=64, you should compile with

```
gfortran -O3 potts.f90 -o potts64
```

where I called the executable `potts64` to distinguish it from the executable with N=32.

Problem 3

Starting from the mathematical definition of the thermodynamical averages, see for instance Eqs. 30 and 31 in my notes on stochastic simulations, demonstrate that the the quantities $< E >$ and C in problem 1 are related by

$$C(\beta) = -\frac{d < E > (\beta)}{d\beta} \tag{1}$$

You should include your derivation of the above identity in a postscript file called assignment8.ps.

Problem 4

Using the data obtained for problem 2, generate the following graph.

1) A single graph displaying the values obtained for $< E >$ versus β in the four simulations. Use points for the results with $N = 32$ and lines for the results with $N = 64$ to make the various results better distinguishable.

2) A single graph displaying the values obtained for C versus β in the four simulations. Use points for the results with $N = 32$ and lines for the results with $N = 64$ to make the various results better distinguishable.

3) A single graph displaying the values obtained for $< m >$ versus β in the four simulations. Use points for the results with $N = 32$ and lines for the results with $N = 64$ to make the various results better distinguishable.

4) A single graph displaying the values obtained for C in the two simulations with $N = 32$ and $N = 64$ and hot start (use points for the values of C) as well as the values for $-d < E > /d\beta$, approximated from the values of $< E >$ obtained in the same two simulations (use lines).

You should include these four graphs in the file assignment8.ps You should use figure captions to distinguish among the four graphs, but do not need to put in any further comments.

Completing and returning the assignment.

For this assignment you must return the modified Potts simulation program, the four output files (see problem 2), a single postscript file with the mathematical derivation requested for problem 3 and the four graphs requested for problem 4.

All of these files must be put together in a single file with the tar command (do not compress the resulting file) and the tar file should be copied on the CAS cluster to the file

~rebbi/courseware/asgn/asgn8.xxyyyy,

where xxyyyy stands for your personal identifier. You can overwrite the file asgn8.xxyyyy as many time as you like until the deadline for the assignment. After the deadline, the write permission on the file will be revoked.

Grading criteria.

25 points will be awarded for a correct solution to each problem, for a maximum score of 100 points. Solutions which contain errors will be given partial credit, according to the severity of the error.