Simulation methods in physics

Homework 3
Return before 13.00 on Tue 4.3., to Ari Hietanen's mailbox (C-wing 3rd floor),
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1. Write a Wolff single-cluster Ising model program in 2 dimensions. (Note that the partition function in the cluster section of the notes is

$$Z = \sum_{\{s\}} \exp[\beta \sum_{<ij>} s_i s_j]$$

i.e. there's a factor of 2 difference in β compared to the previous definition).

Perhaps the easiest way to write the program is to use either the code shown in the lectures (which may be slow due to recursion), or to use the following *width-first* algorithm:

take a random point i as the root of the cluster;
set $s_0 = s_i$;
invert $s_i = -s_0$;
store the coordinate i as the 1st element on a working table (queue);
while (there are elements in the queue) {
    take i =(1st element from the queue);
    for (all neighbours j of i) {
        if ($s_j = s_0$ *and* $1 - e^{-2\beta} > X$) {
            invert $s_j = -s_0$;
            put j at the end of the queue;
        }
    }
}

Here X is a random number $\in [0, 1)$. Since the maximum size of the cluster is V, it is easiest to implement the queue as a table of size V, where one adds elements to one end, and takes them away them from another. Inverting the spin during the growth prevents choosing the same site more than once.

2. Does the algorithm work? Check that you get the same value for energy $E = -\sum_{<ij>} s_i s_j$ at the critical coupling $\beta_c = \ln(1 + \sqrt{2})/2$ than you did using the Metropolis (sorry, should be Heat bath! well, anything goes...) update in the previous exercise (note the factors of 2).

Convert the programs so that you write all energy measurements of the Monte Carlo run on a file. Using both the cluster and Metropolis, perform simulations at $\beta = \beta_c$ on, say, 4–5 lattices of size $12 \leq L \leq 256$, and measure the *integrated autocorrelation time* $\tau_{\text{int.}}$ *of* E. Plot the autocorrelation times against L, and estimate the dynamical critical exponent z: $\tau_{\text{int.}} \propto L^z$. (no fancy power law fitting is necessary, it is sufficient to get a rough estimate for the exponent). What if you measure $\tau_{\text{int.}}$ in units of $cpu - time$ instead of measurements?