Project 15.34. Physical test of random number generators

In Section 7.9 we discussed various statistical tests for the quality of random number generators. In this project we will find that the usual statistical tests might not be sufficient for determining the quality of a random number generator for a particular application. The difficulty is that the quality of a random number generator for a specific application depends in part on how the subtle correlations that are intrinsic to all deterministic random number generators couple to the way that the random number sequences are used. In this project we explore the quality of two random number generators when they are used to implement single spin flip dynamics (the Metropolis algorithm) and single cluster flip dynamics (Wolff algorithm) for the two-dimensional Ising model.

a. Write methods to generate sequences of random numbers based on the linear congruential algorithm
$$x_n = 16807\, x_{n-1} \bmod (2^{31} - 1), \tag{15.81}$$
and the generalized feedback shift register (GFSR) algorithm
$$x_n = x_{n-103} \oplus x_{n-250}. \tag{15.82}$$
In both cases x_n is the nth random number. Both algorithms require that x_n be divided by the largest possible value of x_n to obtain numbers in the range $0 \leq x_n < 1$. The GFSR algorithm requires bit manipulation. Which random number generator does a better job of passing the various statistical tests discussed in Problem 7.35?

b. Use the Metropolis algorithm and the linear congruential random number generator to determine the mean energy per spin E/N and the specific heat (per spin) C for the $L = 16$ Ising model at $T = T_c = 2/\ln(1 + \sqrt{2})$. Make ten independent runs (that is, ten runs that use different random number seeds), and compute the standard deviation of the means σ_m from the ten values of E/N and C, respectively. Published results by Ferrenberg, Landau, and Wong are for 10^6 Monte Carlo steps per spin for each run. Calculate the differences δ_e and δ_c between the average of E/N and C over the ten runs and the exact values (to five decimal places) $E/N = -1.45306$ and $C = 1.49871$. If the ratio δ/σ_m for the two quantities is order unity, then the random number generator does not appear to be biased. Repeat your runs using the GFSR algorithm to generate the random number sequences. Do you find any evidence of statistical bias?

c. Repeat part (b) using Wolff dynamics. Do you find any evidence of statistical bias?

d. Repeat the computations in parts (b) and (c) using the random number generator supplied with your programming language.

Project 15.35. Nucleation and the Ising model

a. Equilibrate the two-dimensional Ising model at $T = 4T_c/9$ and $B = 0.3$ for a system with $L \geq 50$. What is the equilibrium value of m? Then flip the magnetic field so that it points down, that is, $B = -0.3$. Use the Metropolis algorithm and plot m as a function of the time t (the number of Monte Carlo steps per spin). What is the qualitative behavior of $m(t)$? Does it fluctuate about a positive value for a time long enough to determine various averages? If so, the system can be considered to have been in a *metastable state*. Watch the spins evolve for a time before m changes sign. Visually determine a place in the lattice where a "droplet" of the stable phase (down spins) first appears and then grows. Change the random number seed and rerun the simulation. Does the droplet appear in the same spot at the same time? Can the magnitude of the field be increased further or is there an upper bound above which a metastable state is not well defined?

b. As discussed in Project 15.32, we can define clusters of spins by placing a bond with probability p between parallel spins. In this case there is an external field and the proper definition of the clusters is more difficult. For simplicity, assume that there is a bond between all nearest-neighbor down spins and find all the clusters of down spins. One way to identify the droplet that initiates the decay of the metastable state is to monitor the number of spins in the largest cluster as a function of time after the quench. At what time does the number of spins in the largest cluster begin to grow quickly? This time is an estimate of the *nucleation time*. Another way of estimating the nucleation time is to follow the evolution of the center of mass of the largest cluster. For early times after the quench, the center of mass position has large fluctuations. However, at a certain time, these fluctuations decrease considerably, which is another criterion for the nucleation time. What is the order of magnitude of the nucleation time?

c. While the system is in a metastable state, clusters of down spins grow and shrink randomly until eventually one of the clusters becomes large enough to grow, nucleation occurs, and the system decays to its stable macroscopic state. The cluster that initiates this decay is called the nucleating droplet. This type of nucleation is due to spontaneous thermal fluctuations and is called *homogeneous nucleation*. Although the criteria for the nucleation time that we used in part (b) are plausible, they are not based on fundamental considerations. From theoretical considerations the nucleating droplet can be thought of as a cluster that just makes it to the top of the saddle point of the free energy that separates the metastable and stable states. We can identify the nucleating droplet by using the fact that a saddle point structure should initiate the decay of the metastable state 50% of the time. The idea is to save the spin configurations at regular intervals at about the time that nucleation is thought to have occurred. We then restart the simulation using a saved configuration at a certain time and use a different random number sequence to flip the spins. If we have intervened at a time such that the largest cluster decays in more than 50% of the trials, then the intervention time (the time at which we changed the random number seed) is before nucleation. Similarly, if less than 50% of the clusters decay, the intervention is after the nucleation time. The nucleating droplet is the cluster that decays in approximately half of the trial interventions. Because we need to do a number of interventions (usually in the range 20–100) at different times, the intervention method is much more CPU intensive than the other criteria. However, it has the advantage that it has a sound theoretical basis. Redo some of the simulations that you did in part (b) and compare the different estimates of the nucleation time. What is the nature and size of the nucleating droplet? If time permits, determine the probability that the system nucleates at time t for a given quench depth. (Measure the time t after the flip of the field.)

d. *Heterogeneous nucleation* occurs in nature because of the presence of impurities, defects, or walls. One way of simulating heterogeneous nucleation in the Ising model is to fix a certain number of spins in the direction of the stable phase (down). For simplicity, choose the impurity to be five spins in the shape of a + sign. What is the effect of the impurity on the lifetime of the metastable state? What is the probability of droplet growth on and off the impurity as a function of quench depth B?

e. The questions raised in parts (b)–(d) become even more interesting when the interaction between the spins extends beyond nearest neighbors. Assume that a given spin interacts with all spins that are within a distance R with an interaction strength of $4J/q$, where q is the number of spins within the interaction range R. (Note that $q = 4$ for nearest neighbor interactions on the square lattice.) A good choice is $R = 10$, although your preliminary simulations should be for smaller R. How does the value of T_c change as R is increased?

Project 15.36. The n-fold way: Simulations at low temperature

Monte Carlo simulations become very inefficient at low temperatures because almost all trial configurations will be rejected. For example, consider an Ising model for which all spins are up, but a small magnetic field is applied in the negative direction. The equilibrium state will have most spins pointing down. Nevertheless, if the magnetic field is small and the temperature is low enough, equilibrium will take a very long time to occur.

What we need is a more efficient way of sampling configurations if the acceptance probability is low. The *n-fold way* algorithm is one such method. The idea is to accept more low probability configurations, but to weight them appropriately. If we use the usual Metropolis rule, then the probability of flipping the ith spin is

$$p_i = \min\bigl[1, e^{-\Delta E/kT}\bigr]. \tag{15.83}$$

One limitation of the Metropolis algorithm is that it becomes very inefficeint if the probabilities p_i are very small. If we sum over all the spins, then we can define the total weight

$$Q = \sum_i p_i. \tag{15.84}$$

The idea is to choose a spin to flip (with probability one) by computing a random number, r_Q, between 0 and Q and finding spin i that satisfies the condition:

$$\sum_{k=0}^{i-1} p_k \le r_Q < \sum_{k=0}^{i} p_k. \tag{15.85}$$

There are two more ingredients we need to make this algorithm practical. We need to determine how long a configuration would remain unchanged if we had used the Metropolis algorithm. Also the algorithm would be very inefficient because on average the computation of which spin to flip from (15.85) would take $O(N)$ computations. This second problem can be easily overcome by realizing that there are only a few possible values of p_i. For example, for the Ising model on a square lattice in a magnetic field, there are only $n = 10$ possible values of p_i. Thus, instead of (15.85), we have

$$\sum_{\alpha=0}^{i-1} n_\alpha p_\alpha \le r_Q < \sum_{\alpha=0}^{i} n_\alpha p_\alpha, \tag{15.86}$$