Simulating and Visualising Phase Transitions: Small-World Effects on the Monte Carlo Ising Model

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The Ising Model

Many physical, social, and technical systems exhibit phase transitions or other critical behaviour. A phase transition occurs in a system when a small change in some parameter of the model or system leads to a dramatic change of some characteristic property. The system or model is said to have changed phase. A well known physical example is a magnet which exhibits magnetism up to a critical temperature, above which its magnetic properties are suddenly destroyed. Similarly, on cooling a material such as iron, the spins of individual atoms will organise themselves spontaneously into alignment below the critical temperature and the material becomes magnetic. A simulation model such as the Ising model has been widely used to study this sort of phase transition. An energy coupling model is established between nearest neighbouring spin bits on a lattice mesh, and a Monte-Carlo quench experiment from a random initial configuration (representing an infinite temperature) is performed to produce giant clusters of like-like spin bits below and around the critical temperature. The model can be used to find the critical temperature in 2-, 3-, and 4-dimensions. If random lattice re-wirings are applied to the lattice, the effect of small-world network perturbations can also be studied.

The Ising model is usually formulated on a regular d-dimensional hyper-cubic lattice where each magnetic spin variable is connected to its $2 \times d$ nearest-neighbouring sites. The energy Hamiltonian is written in the form:

$$H = -\sum_{i \neq j} J_{ij} S_i S_j \qquad (1)$$

where $S_i = \pm 1$, $i = 1, 2, ...N$ sites, and J_{ij} is $|J| = 1/k_B T$ is the ferromagnetic coupling over neighbouring sites i,j on the network.

The model has a critical temperature of $T_c = \frac{1}{J_i k_B} = 0$ in one dimension, but displays finite transition temperatures due to the spontaneous magnetization effects in higher dimensions. Specifically in two- and three-dimensions the Ising-type phase transitions have been very well studied and the critical temperatures are known exactly in two dimensions [1] and approximately from computer simulations such as [2] in three dimensions. In systems of four dimensions and higher a finite temperature phase transition still occurs, but the nature of the transition is well described by mean-field theory. Values for the transition temperature in these higher dimensional systems and under special conditions are also known although the amount of computational work and number of simulations needed to calculate these values can be considerable.

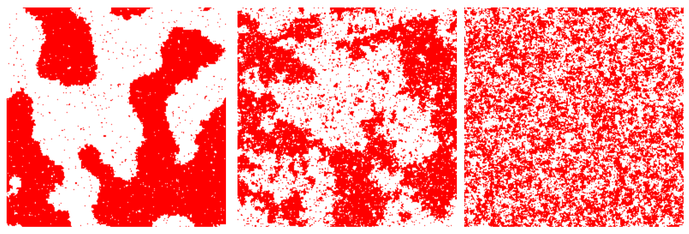

Figure 1: Cold, Critical and Hot Ising Configurations

The figure shows a 256×256 regular lattice Ising model, initialised as a "infinitely hot" random mixture of spin-up and spin-down sites, and subsequently quenched to a finite temperature below, around or above the critical temperature. Below this, the system undergoes a phase transition, the spins spontaneously align and the system becomes a magnet.

The regular lattice Ising model can be perturbed in a number of controlled ways: by removing bonds or "damaging" the system; by re-wiring the bonds; or by adding extra bonds. Herrero and others have employed the Watts-Strogatz re-wiring model which preserves the number of total bonds, but does not preserve the number of bonds connecting a given site. Svenson and Johnson explored damage spreading in small-world Ising systems [3], again using the Watt-Strogatz approach.

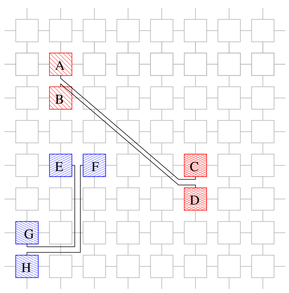

Figure 2: Re-wiring a 2-D Regular Lattice while still preserving the number of links for each site as $2 \times d = 4$.

Generally, the Ising model phase transitional temperature is systematically shifted by these damaged, rewired or added links[4, 5]. In the case of the small-world re-wiring, individual sites can become connected to sites very far away physically. These long-range bonds encourage and help the long-range correlations that manifest the spontaneous magnetization and hence give rise to the peculiarly Ising-like critical phenomena. The Ising model critical temperature rises as long-range order is encouraged by the re-wiring. Physically, it is easier for the system to maintain long-range order against the thermal disordering effects of higher temperatures than it would be without the rewired long-range bonds. This can be measured as a monotonic dependence of the critical temperature $T_c(p)$ on the small-world re-wiring probability p.

Locating Critical Temperatures

We compute the temperature shift $\Delta T_c = T_c^p - T_c^{p=0}$ based on the critical temperature measured for a small-world rewired Ising model system, compared with that of an unperturbed system on a regular lattice.

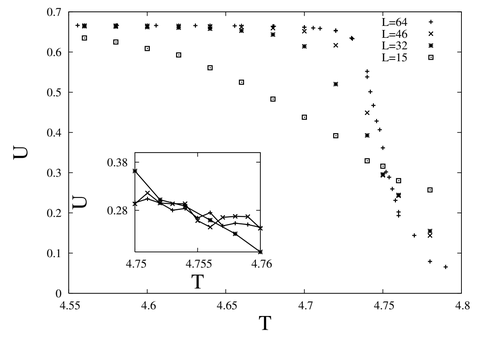

Figure 3: Binder Cumulants - S-shaped curves that intersect at the critical point.

The critical temperature of a Monte Carlo simulated system can be calculated using the fourth-order Binder cumulant method [6, 7]. The cumulant:

$$U_N = 1 - \frac{\langle M^4 \rangle_N}{3 \langle M^2 \rangle_N^2} \qquad (2)$$

is defined at different network sizes N, where $N = L^d$ based on the edge length L of our substrate lattice. The cumulant shows a transition edge at the critical temperature. The cumulant curves for different N (or L) values coincide at the critical temperature and this gives a way of extrapolating to the thermodynamic limit from relatively small sized simulations. Figure 3 shows the form of the cumulant and how it has a sharper transition edge at larger system sizes. A practical method of obtaining a critical temperature is to simulate at least three different system sizes and by fitting straight lines to the linear region of the cumulant curve around the critical temperature, calculate the intercept and an uncertainty estimate. For all the work we report in this paper we used at least three system sizes. For small systems multiple independent re-wiring configurations can be sampled. For very large systems needed for estimating low-p behaviour it is impractical to run more than a few independent samples and consequently the measurement uncertainties are very much greater. We can estimate the critical temperatures for two- and three-dimensional systems to around four significant figures and to three significant figures for four-dimensional systems. Our five-dimensional system simulations are limited to qualitatively showing that a small-world effect takes place.

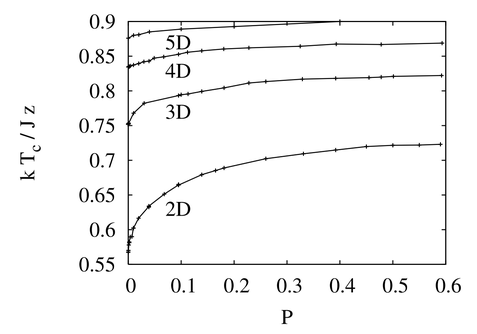

Figure 4: Variation of Critical Temperature with Re-wiring probability

Generally, obtaining the shifted critical temperatures for different p-values was an iterative procedure. We employed small lattice sizes to home in on approximate locations then used progressively larger system sizes to refine precision and uncertainties. Figure 2 shows the qualitative behaviour of the critical temperature as it varies with p for different dimensionalities.

Analysis of the shift $\Delta T_c = T_c^p - T_c^{p=0}$ in the critical temperature (see figure 4) from the regular lattice value of shows a power law of the form $\Delta T_c^{(p)} \approx p^s$. This confirms that well below the percolation limit, where the system is essentially one single component, the behaviour is independent of the re-wiring model.

Making it Fast

The finite size effects that blunten the phase transition can only be combatted if we can make the system simulation size as large as possible. In this work we were limited by the memory available on a typical computer. Although the spins in the model can be stored as single bits - accessing a single bit packed into 32- or 64-bit words is quite slow and it is faster if we store spins as a whole `byte` or even a whole `word` or `int`. The rewired lattice needs to have a complete set of neighbours stored as a graph and this adds to the storage - since each node needs 4 `ints` stored for a 2-d model, or 6 for a 3-d model. We found practically that for 32-bit processor architectures limited to 2GBytes of storage memory, we could manage a $384 \times 384 \times 384$ lattice at the largest.

To thermally equilibrate a system of this size would take several weeks of computer runtime, using conventional Monte Carlo algorithms. Since we needed to run at least 100 separate configurations at each temperature and re-wiring probability this would have been in feasible even with a supercomputer cluster at our disposal. We were able to partition all the different runs into multiple jobs that ran on Massey's Helix supercomputer cluster - taking several processor years in total to harvest all the necessary data and taking several months just to combine all the averages and fit the appropriate statistics.

The Monte Carlo lattice simulation method works fairly simply for models like the Ising system. The procedure is:

1. Pick a spin site in the lattice at random;
2. Work out what would happen to the energy E of the whole system if that spin was "flipped";
3. If energy drops accept the change, but if energy would rise accept the change with a conditional probability - computed by comparing a random number with the Boltzmann energy factor $e^{-\Delta E/kT}$.
4. Repeat from 1.

We apply this "Metropolis Monte Carlo" procedure for many iterations so the spin system equilibrates. A faster procedure involves occasionally identifying an entire cluster of spins and flipping them. This is known as the Wolff cluster algorithm and speeds up the equilibration process considerably. We employed a hybrid Wolff/Metropolis procedure for our work.

Computer generated random numbers are obviously crucial to this algorithm. We need fast random numbers that can be computed on a supercomputer - but they need to be good ones - that is they must not be correlated as that would bias the calculations and come up with the wrong answer for the critical temperature. We used Marsaglia's lagged Fibonacci generator for the work reported here. This is a very fast generator that is almost as good quality as the slightly slower Mersenne Twistor generator. The latter is a 64-bit algorithm and as 64-bit processors replace 32-bit architectures, the Mersenne Twistor random number generator will be the algorithm of choice for this sort of work.

Discussion and Conclusions

We studied both the Watts-Strogatz and our z-preserving re-wiring models in detail on small-world systems constructed from 2-D, 3-D and 4-D hyper-cubic lattices. For each dimension we studied at least three decades of p values and in the case of 3-D systems we studied six decades of p down to 10^{-6} on systems of up to $N \approx 384^3$. A preliminary study of a 5-D system also indicates that the small-world shift in T_c does take place, although our 5-D data is as yet insufficient to determine a useful value of s.

For $p \lesssim 0.1$ we are below the percolation regime and the system consists of one large component for the W-S model. In this regime our re-wiring model and the W-S re-wiring model are in agreement within the limits of experimental error, and furthermore agree closely with the 3-D data reported for a W-S re-wiring model [8]. Combining all data we find $s \approx 0.698 \pm 0.002$. Although we have less data for 2-D systems, we investigated larger system sizes (up to 1024^2) than Herrero, and do not find the tail-off he reports for small-p. We find a very good fit for $s \approx 0.50 \pm 0.001$ for 2-D systems.

We conclude that the $\Delta T_c^{(p)} \approx p^s$ power-law is a very good description of all the data and any deviation from it is indeed due to finite-size limitations that do not properly achieve the small-p regime as Herrero correctly suggests for his data.

This model is proving a useful theoretical and computational tool for exploring the implications of small-world shortcuts on systems that exhibit phase transitions. Simulations of this model do require investigation over many time and space scales and over several logarithmic decades of the re-wiring probability parameter. For this reason, supercomputers, parallel resources and several sophisticated algorithmic tricks are all necessary to achieve practical results.

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