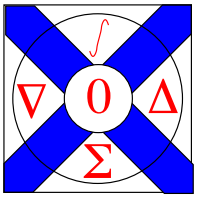

Computational Science Technical Note **CSTN-006**

Fast Monte Carlo Algorithms on Re-Wired Small-World Spin Models

K. A. Hawick

2009

Small-world networks have become an important model for understanding many complex phenomena in science and in sociological contexts. One tool for exploring the critical and phase transitional behaviour in small-world systems is to simulate known models on grids and networks that have been re-wired using the small-world approach. A well known model for studying phase transitions is the Ising spin model. This system is usually studied using an artificial Monte Carlo dynamics scheme and for the study of large model systems fast update algorithms based on whole cluster updating are necessary. These algorithms can not be applied to arbitrarily re-wired models. In this paper we apply a special pair-wise re-wiring that conserves the number of connected neighbours of each spin site and to which fast cluster update algorithms can be applied. We describe the algorithm and its implementation and present some convergence results which are compared with those from more traditional Monte Carlo approaches.

Keywords: Monte Carlo; dynamics; small-world; network; Ising

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Fast Monte Carlo Algorithms on Re-wired Small-World Spin Models

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Abstract

Small-world networks have become an important model for understanding many complex phenomena in science and in sociological contexts. One tool for exploring the critical and phase transitional behaviour in small-world systems is to simulate known models on grids and networks that have been re-wired using the small-world approach. A well known model for studying phase transitions is the Ising spin model. This system is usually studied using an artificial Monte Carlo dynamics scheme and for the study of large model systems fast update algorithms based on whole cluster updating are necessary. These algorithms can not be applied to arbitrarily re-wired models. In this paper we apply a special pair-wise re-wiring that conserves the number of connected neighbours of each spin site and to which fast cluster update algorithms can be applied. We describe the algorithm and its implementation and present some convergence results which are compared with those from more traditional Monte Carlo approaches.

Keywords: Monte Carlo; dynamics; small-world; network; Ising.

1 Introduction

Complex networks [1] based on small-world re-wiring properties [2] are now an important class of complex system and have been used for many purposes ranging from social network models [3] to quantum gravity [4].

An important characteristic of the small-world network or graph model is that it allows a parameterized interpolation between those properties exhibited by a random graph [5] and those by regular lattices. A re-wiring probability p can be varied quantifiably between 0 and 1. Understanding the process that lead to small-world networks is non-trivial [6, 7] and one important approach involves comparing the critical phase transitional behaviour of small-world systems with well-studied phase transition models. The Ising model provides a valuable test model for studying phase transitions on various networks. Study of the 1-D Ising model [8] has led to some insights and relatively recent work by Herrero [9,10] and others [11] raises some interesting questions about the behaviour of the Ising model on small-world re-wired lattices.

The anomalous scaling behaviour of the Ising model on small-world networks causes a shift in the critical temperature that scales as p^X for re-wiring probability p and some exponent x that can be determined experimentally from simulations. To explore this in the thermodynamic or large-scale limit requires simulation of a range of large network models. Unfortunately there is an often-encountered phenomena in phase transitional systems known as critical slowing down [12]. Near the critical temperature (which is the parameter area we want to study) the dynamics causes an intrinsic slowing down and it is necessary to employ some sophisticated cluster update algorithms to accelerate the Monte Carlo sampling and hence avoid infeasably slow simulation times. Traditional Monte Carlo algorithms for studying models such as the Ising system can be easily applied to re-wired model systems but do suffer from this slowing down effect.

In this paper we apply fast cluster update algorithm such as that of Wolff to a special pair-wise small-world re-wiring model. In section 2 we present the Ising spin model and discuss how it can be used as a tool to study the changes in phase transitions in small-world re-wiring models in section 3. We discuss Monte Carlo

update algorithms in section 4 and present some convergence results in section 5. We discuss the implications for large scale simulation models and offer some conclusions in section 6.

2 The Ising Spin Model

The Ising model is usually formulated in terms of a set of single bit spin variables $S_i$that are arranged on a network or graph of N sites. Usually the graph is a simple square or simple cubic lattice, with each spin coupled though a parameter J to its nearest neighbours. The coupling is essentially the same as an inverse temperature, and there is a critical value of this temperature above which the spins all behave randomly. At cold temperatures below the critical temperature the spins align and the system becomes a magnet. The critical temperature effect is seen in real materials - in iron for example it is known as the Curie temperature. Heat a bar magnet above this temperature and all its magnetism is destroyed.

We employ the usual nearest neighbour Ising Hamiltonian to describe the energy of the model: $H = -\sum_{i,j} J_{ij} S_i S_j$ 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.

Although the Ising model does not have a dynamics of its own, an artificial dynamics in the form of one of the variations of the Markov Chain Monte Carlo(MCMC) update algorithms can be interpreted in terms of a simulation time. Investigations of the MCMC method in various contexts have shown that under certain conditions, MCMC simulation time does correlate and scale appropriately in a manner consistent with real physical systems' time [13]. The bond topology distortions described below provide a means for information to propagate faster across the lattice during a simulation.

A conventional MCMC update approach will apply approximately one "hit" per site in a complete time step. Generally, on average, it will therefore take $O(L/2)$ steps for information to propagate across a lattice with edge length L. The factor of two is from likely periodic or wraparound boundary conditions. One or more "worm-holes" applied as in figure1 will allow changes in one site to propagate across long distances in considerably shorter times. The effect of the swapped bond pairs can therefore be interpreted as either making sites closer to one another in a distorted space metric, or as providing special "fast conduits" or "worm-holes" across which information can propagate more quickly than elsewhere on the lattice.

The update schemes to make the spins change in time are discussed in section 4 below.

3 Small-Worlds

Many computational physics models are formulated on a regular mesh or on a topologically regular system. For example the familiar square, cubic or hyper-cubic geometries have sites with 4, 6 or 8 nearest neighbouring sites. If the systems have periodic boundary conditions then it is possible to assign unique "ownership" of half of the bonds or links to a particular site. So each site of the square lattice has 2 bonds that can be uniquely associated with it. The lattices can be considered as graphs with twice as many edges as there are nodes.

It seems likely that many of the familiar properties of models such as the Ising [14], Potts [15] or Heisenberg [16] models depend on the geometry of the underpinning lattice. An interesting question is to ask how strong this dependence is upon local properties such as number of neighbours as against the actual geometry itself. For instance, we can construct a lattice which has the same topology as the conventional square mesh and where each site will still have 4 neighbouring sites, but where the layout is no longer trivial. Such a lattice can be constructed by making pairwise perturbations to a conventional square mesh. A question of interest is, at what point, if any, the behaviour of the Ising model changes as a function of the number of changed bonds?

The effect of these connectivity "worm-holes" will allow information to propagate across long ranges or an alternative interpretation is the speed of propagation of information is increased. Intuition suggests that this long range communication mechanism will encourage long range order and thus raise the critical temperature of the system. Interpretation of the geometry of such a model is non-trivial. What does it mean for the model's physical space to be interconnected in such a manner? The axes and dimensions of the model are effectively inter-folded or mixed and these models provide a useful tool to explore these questions.

Our network is constructed from the starting lattice using a re-wiring procedure. We modify the bonds of each site so that it still has degree $2 \times d$ bonds per site in dimension d, but that they may link, with probability p, to a randomly chosen site elsewhere in the original lattice. We ensure each site links to other sites at most once, and there are no self-bonds in our system. This is feasible below the percolation threshold.

Figure 1 shows the essence of our re-wiring algorithm. The essence of our procedure is:

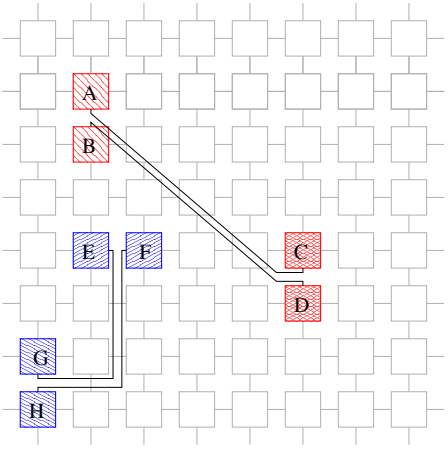

Figure 1: Small-World z-conserving re-wiring model on a 8 by 8 lattice.

- choose a random bond (by choosing a random site A and one of its bonds) which connects to neighbouring site B
- randomly choose another (distinct) site C and one of its bonds, which connects to neighbouring site D
- effectively swap bonds $A-B$ and $C-D$ to obtain bonds $A-C$ and $B-D$

Figure 1 shows this for bonds $A-B$, $C-D$, $E-F$ and $G-H$. Swapping bonds in pairs like this ensures we always preserve the lattice coordination number z. Note that $z = 2d$ for regular hyper-lattices.

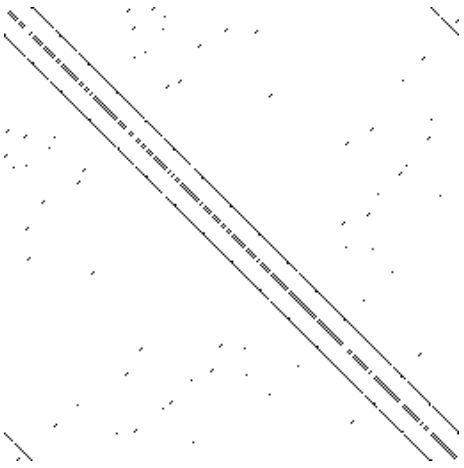

Figure 2: Adjacency matrix for a 16x16 lattice with small world re-wire probability $p = 0.1$.

Figure 2 shows the adjacency matrix for a re-wired lattice. The main diagonal and off diagonal lines correspond to the nearest neighbour links. These are gradually removed and appear as arbitrary links as the re-wire probability p is increased. To properly explore the parameter space of p it is necessary to use large networks sizes N so that $pN > 0$.

4 Update Algorithms

Modern works studying critical systems like the Ising model use the Monte Carlo Renormalisation Group method [12, 17]. This method unfortunately does not extend in an obvious way to perturbed lattice model systems. A number of cluster-based Monte Carlo updating algorithms followed from the work of Swendsen and Wang [18] including the Wolff algorithm [19] we employ. These works have given rise to specialised cluster identification methods [20], [21] and discussions of the effectiveness of the Wolff algorithm [22].

We now present a derivation of the appropriate transition probabilities for the Monte-Carlo dynamics and review how the Monte Carlo update algorithm arises.

Each microstate of the Ising system is completely specified by the set of site variables $\{s_i\}$ given the coupling. Let the probability functional $P(\mathbf{X}, t)$ be associated with the microstate $\mathbf{X} \equiv \{s_i\}$ at time t and consider the transition probability $W_{\mathbf{X}\to\mathbf{X}'}$ giving the likelihood of a change of microstate $\mathbf{X}$ to $\mathbf{X}'$. The following master equation can immediately be set up, requiring that the rate of change of probability of microstate $\mathbf{X}$ at time t be given by considering all transitions from $\mathbf{X}$ and all transitions to $\mathbf{X}$:

$$\frac{dP(\mathbf{X})}{dt} = -\sum_{\mathbf{X}'} W_{\mathbf{X}\to\mathbf{X}'} P(\mathbf{X}) + \sum_{\mathbf{X}'} W_{\mathbf{X}'\to\mathbf{X}} P(\mathbf{X}') \quad (1)$$

By requiring the algorithm to yield $P(\mathbf{X}) \to P_{eq}(\mathbf{X})$, the thermodynamic equilibrium probability of microstate $\mathbf{X}$ as $t \to \infty$ a solution of 1 with $\frac{dP(\mathbf{X})}{dt} = 0$ so that:

$$\sum_{\mathbf{X}'} W_{\mathbf{X}\to\mathbf{X}'} P(\mathbf{X}) = \sum_{\mathbf{X}'} W_{\mathbf{X}'\to\mathbf{X}} P(\mathbf{X}') \quad (2)$$

This is the condition of detailed balance. It is common to use the stronger (but tractable) condition that:

$$\frac{W_{\mathbf{X}'\to\mathbf{X}}}{W_{\mathbf{X}\to\mathbf{X}'}} = \frac{P(\mathbf{X})}{P(\mathbf{X}')} \quad (3)$$

So that the probability of the system moving to microstate $\mathbf{X}$ is increased for highly probable microstates

X, and decreased for unlikely ones. It is then necessary to recognize that for a Boltzmann statistical weighting of the microstates, the probabilities $P(\mathbf{X}$ can be expressed in terms of the Hamiltonians $\mathcal{H}(\mathbf{X})$.

$$P(\mathbf{X}) = Ae^{-\frac{\mathcal{H}(\mathbf{X})}{k_b T}} \tag{4}$$

Where A is a normalising constant, k_b is Boltzmann's constant and T the temperature. Substituting 4 in 3 gives:

$$\frac{W_{\mathbf{X}'\to\mathbf{X}}}{W_{\mathbf{X}\to\mathbf{X}'}} = e^{-\frac{\{\mathcal{H}(\mathbf{X})-\mathcal{H}(\mathbf{X}')\}}{k_b T}} \tag{5}$$

This does not have a unique solution. We seek a practical microstate updating algorithm expressed in terms of:

$$\triangle\mathcal{H} = \mathcal{H}_{X'} - \mathcal{H}_X \tag{6}$$

which allows us a practical way of computing the transition probability from X to X'. The two most commonly used are the Metropolis algorithm [23]:

$$W_{\mathbf{X}\to\mathbf{X}'} = \begin{array}{ll} \frac{1}{\tau}e^{-\frac{\triangle\mathcal{H}}{k_b T}}, & \triangle\mathcal{H} > 0 \\ \frac{1}{\tau}, & \triangle\mathcal{H} \leq 0 \end{array} \tag{7}$$

and the Glauber algorithm [24]:

$$W_{\mathbf{X}\to\mathbf{X}'} = \frac{1}{\tau}\left(\frac{e^{-\frac{\triangle\mathcal{H}}{k_b T}}}{1+e^{-\frac{\triangle\mathcal{H}}{k_b T}}}\right) \tag{8}$$

It remains to decide which of these two schemes produces the more realistic dynamics. Older works in the literature such as [24] have used the Glauber scheme for dynamical work, relegating the Metropolis algorithm to work where a thermodynamically equilibrated configuration is required and the dynamics is unimportant.

It appears that for computational purposes, the Metropolis algorithm is better, since it involves one less floating point operation – a division, it produces a faster dynamics but similar equilibrium results, and a qualitatively similar trajectory through phase space.

The simulation time can then be defined in units of 'an average of one Metropolis update attempt per site'. It is important to include every site in this definition of the time-step. Without such a universal definition, it becomes impossible to compare other works in the literature and on slightly different models, in terms of their dynamical properties. The problem remains that this is only an artificially constructed time. It is also noticeable that for deep quench experiments, there is little thermal activity below the phase transition temperature and the system evolves very slowly. This effect is known as hydro-dynamic slowing down.

The Metropolis Monte Carlo algorithm is but one of various possible Markov Chain approaches to the exploration of the phase space of a model like the Ising system. Various authors have proposed alternatives and there is still discussion on the validity and usefulness of various Monte Carlo algorithms, including the vexatious question of the significance of detailed-balance and sequential updates. See for example [25], [26], [27] [28], [29], [30].

A number of new Monte Carlo algorithms have appeared recently in the literature, purporting to speed up the dynamics and reduce the effect of the hydrodynamic slowing down. Some of these are [31], [32], [18], and are reviewed in [33] and [34]. In general, they are all short-cuts to finding the most thermodynamically probable region of phase space, and thus are excellent for obtaining thermally equilibrated configurations.

The Wolff algorithm [34] involves constructing a "cluster" of like spins and potentially flipping the spin sign of this entire cluster. In consequence, this algorithm traverses micro-state space in larger "jumps" than either the Metropolis or Glauber update algorithms. This is particularly important in model of critical phenomena like the Ising model whereupon the Wolff algorithm does not suffer from the critical slowing down phenomenon that typically plagues other simulation algorithms near the critical temperature.

The key feature of the Wolff algorithm's ability to meet the detailed balance condition in equation 2 is the precise way that clusters are constructed.

The Wolff algorithm, is essentially:

- Pick a random lattice site, i, as the first point of a cluster to be built
- Flip spin s_i and remember i
- Visit all links connecting site i to its nearest neighbours j
  - The bond $i-j$ is activated with probability $1-e^{\min(0,2\beta)}$
  - Where this happens s_j is flipped and site j is marked as part of the cluster
  - Continue this process for all bonds leading to unmarked neighbours until the process stops
- Ergodicity is guaranteed since there is always a non-vanishing probability that the cluster consists of only one site.

The implications of this algorithm are that a Wolff cluster being constructed as part of the time-evolution of

the system is bounded in size by the extent of the physical cluster in which the initial random site is chosen. We believe the size distribution of Wolff clusters is closely related to the physical cluster size distribution for systems in equilibrium.

5 Cluster Results

There are several important time-scales we must consider when planning a simulation of the Ising model. Generally speaking, the work we discuss here involves infinite quenching experiments. We initialise the system from a "hot" or completely random mixture of "up" and "down" spins. The system is then evolved to thermal equilibrium for a finite temperature T. Once the system has reached equilibrium it is valid to measure macroscopic properties from individually sampled microstate configurations. Realistic statistical averages are obtained providing these samples truly represent the equilibrium properties of the system and also that they are sufficiently decorrelated so as not to introduce a systematic bias.

Consequently it is important that simulations be run for long enough that they are truly in thermal equilibrium for the quench temperature T. Figure 3 shows the approach to equilibrium achieved by the Metropolis, Glauber and Wolff algorithms on the Ising model at critical temperature T_c. The curves show the behaviour of the system's total energy E as it converges to an equilibrium value. Subsequently variables such as E will fluctuate around a mean thermal average value. It is important to distinguish between the equilibration period and the equilibrated regime.

To obtain statistically independent or decorrelated samples it is important that the update algorithm provide an efficient means for the system to traverse its micro-state space at equilibrium.

The total model system energy can be tracked with update time and this is shown in 3. The Glauber algorithm is not appreciably different from the Metropolis algorithm for our system. The Wolff algorithm is however. The Wolff algorithm is based on flipping a whole cluster of like spins. As can be seen, when the system is hot (random) during its initial quench, the Wolff algorithm changes the system energy very slowly. This is because there are only very small clusters present initially. Gradually, the Wolff algorithm "picks up speed" as larger clusters form, and eventually it is able to flip cluster comparable in size to half the system size or more at once.

An obvious conclusion from this is that a hybrid algorithm is optimal. A few Metropolis steps at the early stages can rapidly move the system from hot small clusters to having an appreciable number of large enough clusters so that the Wolff algorithm can do its job effectively. Wolff then cuts in and rapidly moves the system in phase space to give good decoupled configuration samples that do not manifest the critical slowing down.

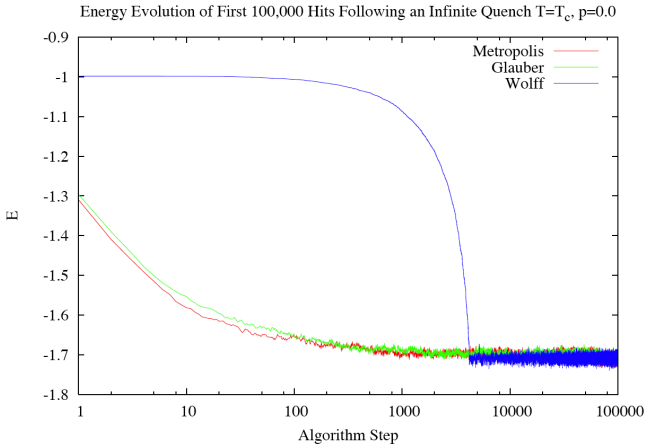

Figure 3: Different equilibration rates for Metropolis, Glauber and Wolf algorithms on a smallish 2D Ising system.

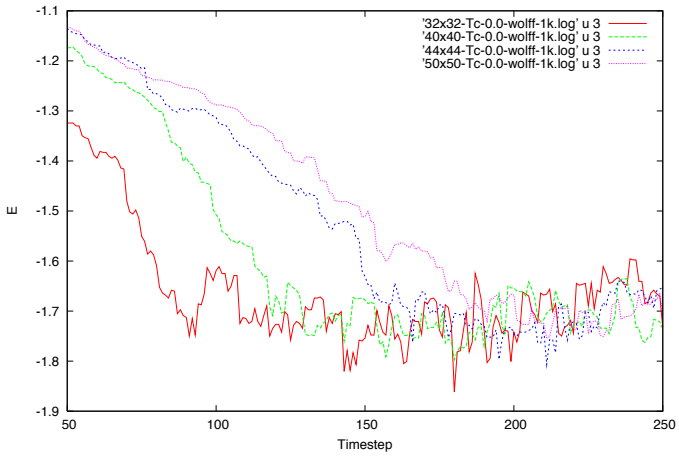

Figure 4: A more fine-grained variation of the timesteps towards equilibration of energy for the Wolff algorithm at different 2D lattice lengths.

Figure 4 shows a more fine grained analysis of the time convergence of the Wolff algorithm as the system size is varied. The larger the system the longer it takes to settle as might be expected. However note that after a mere few hundred steps some sort of equilibration has been reached by the Wolff algorithm.

The histogrammed energy values of the system also provides a quantifiable means of comparing the different

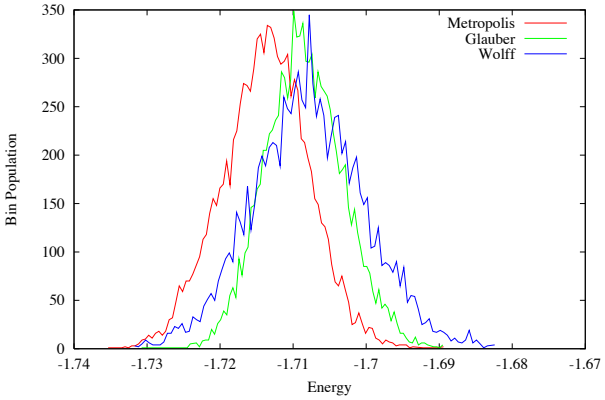

Figure 5: The histogrammed energy values from the last 10,000 algorithm "hits" in a sequence of 100,000 hits in total.

update algorithms. This is illustrated in figures 5. The signature of energy values has the same distribution shape for all three algorithms, although this shows the slow convergence of the Metropolis system as after the stated 10,000 steps the system has not yet reached the same mean peak value as when Wolff and Glauber are used.

Some further results concerning the measured shifts in the critical temperature are presented in [35]. These seem justifiable based on the confirmed convergence behaviours shown in this present paper.

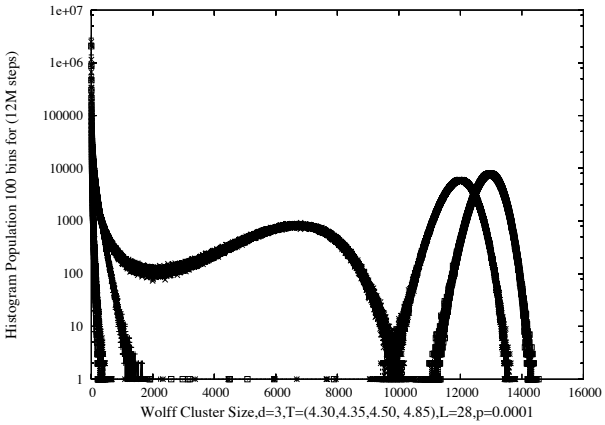

Figure 6: Histogrammed Wolff number W_N for 3D, L=28, T=4.30, 4.35, 4.50, 4.85, p=0.0001

Figure 6 shows the histogrammed values for the Wolff cluster number W_N for a temperature below, near and above the critical temperature, and with small probability p of small-world re-wiring. At high temperatures the distribution of clusters in the system is a long tailed exponential, with predominantly small clusters. At low temperatures the giant super-cluster dominates and the distribution has a peak at some large but finite cluster size, it drops to zero at mid ranges and joins to the exponential distribution with maximum at monomer clusters. A cross-over occurs at the phase transition, and the peak only appears at temperatures below the critical temperature.

6 Discussion and Conclusions

We have discussed how different Monte Carlo update algorithms can be applied to an Ising model spin simulation on re-wired lattices. We have implemented the Wolff whole-cluster update algorithm which is sensibly defined providing we have a consistent energy Hamiltonian which we base on pair-wise small-world re-wiring.

We have studied systems in 2, 3 and 4D and and have been able to obtain better statistics since we have used the Wolff cluster updating method [35]. This does however raise some interesting philosophical issues about what a spatial cluster means in the re-wired lattice model. A cluster can be constructed to span parts of the lattice that are connected through worm-holes and the whole thing is no longer very physical. Nevertheless as an algorithm the system and model is interesting and we have sought to see if we can reproduce Herrero's result and extend it in higher dimensions.

We can conclude that the Wolff algorithm does work sensibly on our re-wired lattice, and produces energy convergence and distribution results that are consistent with better understood traditional Monte Carlo algorithms on small-world re-wired lattices. We observe that a hybrid of Metropolis and the Wolff algorithm is best at least in the early stages of the quench experiment to find the critical temperature. The hybrid allows clusters to form rapidly and for subsequent Wolff hits to be maximally effective.

Our system with a conserved number of neighbours z appears to be intrinsically interesting and to provide another tool for exploring criticality and the effects of folded space and dimensionality in small-world network models.

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