The Effect of Defects on the Ferromagnetic Ising and Antiferromagnetic Cubic Lattice Potts Models

By
Michael Thomas Clauss
Department of Physics
Allegheny College
Meadville, Pennsylvania

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Dr. Shafiqur Rahman	**Date**	**Dr. Jamie Lombardi**	**Date**

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Name: Michael Thomas Clauss Date: Spring, 2017
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Thesis Committee: Dr. Shafiqur Rahman, Dr. Jamie Lombardi
ABSTRACT

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The Potts model is a statistical model that can be useful in simulating a wide range of systems. This can include biological systems, social systems, neural networks, migratory patterns, liquid-gas phase transitions, and many others. However, none of these systems exist in real life without some level of inherent imperfections. The original source-code for an antiferromagnetic Potts model on a simple cubic lattice was modified to include random defects. This allows for a more accurate application of the model to real world systems. Effects of these defects on the transition temperature between the ordered and the disordered phases are discussed.

1 Introduction:

1.1 Summary of Models:

In its beginning, the Potts model was thought to be an order-disorder transitions system of purely theoretical value [Wu, 1982]. As it turns out, it is a statistical model that has given us much insight into many physical systems, both natural and human-made, as well as social systems. However, no real life system exists without defects, and because of this, it is important to have a model that considers defects. Studying a Potts model that includes defects will make it more applicable to a wider variety of applications as a method of statistical analysis through simulation [Zheng *et al.*, 2015]. However, the Potts model did not simply appear out of someone's imagination; it was born of the simpler, more focused, Ising model.

1.1.1 Ising Model:

The Ising model was first developed as a way of studying magnetism based on spins, and was completed in 1925 [Fitzpatrick, 2006]. This model has discrete elements and can be of one or more dimensions. For one, two, and three dimensions, the structure is that of a line, a planar lattice, and any three-dimensional shape that can be represented by a lattice structure. Each element of the lattice has q possible orientations, and in the case of the Ising model $q = 2$, which is demonstrated in Figure 1. The total energy of the lattice can be calculated, when given a specific set of orientations by the Hamiltonian [Gould and Tobochnik, 1986].

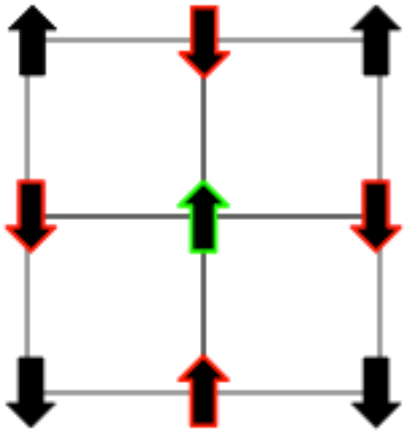


Figure1: Diagrammatic representation of the 2-dimensional Ising Model. Each element has two possible orientations (up or down). Each element on interacts with its nearest neighbors. For example, the element shown with green outline interacts with the ones shown with red outline.

$$H = -J \sum_{<i,j>} s_i s_j \qquad (1)$$

$$J \equiv Exchange\ Energy\ ;\ <i,j> \equiv Nearest\ Neighbor\ indices\ ;\ H \equiv Hamiltonian\ (Energy)$$

$$;\ s_{i/j} \equiv Spin\ orientation\ of\ specific\ element, can\ be\ +1\ or\ -1$$

Computer simulation, specifically the Markov Chain Monte Carlo technique, allows this lattice energy as well as other quantities, such as magnetization, to be calculated quickly

and repeatedly [Chen *et al.*, 1995], and then averaged to provide information about the critical behavior of the system.

1.1.2 Potts Model:

Potts model is a generalization of the Ising model in that it can be applied to a greater range of systems such as foam behaviors, biological membranes, social behavior, spin glass [Harris, 1974], neural networks, flocking birds, and liquid-gas transitions [Ellis, 2006]. The work of Somorjai (1973) and Domany *et al.* (1977) demonstrated that the four state Potts model can simulate the transitions of monolayers and sub-monolayers adsorbed on crystal surfaces. Domany *et al.* (1977) helped to group square, triangle, and honeycomb lattices into the four-state Potts model universality and suggested that N_2 adsorbed onto krypton-plated graphite would exhibit behavior as a four-state Potts model [Wu, 1982]. These discoveries are not focused on defects within the model, but rather on the practical applications of the Potts model. The critical behavior of the Potts model is far richer than that of the Ising model because it allows for more than two possible element orientations, or $q > 2$ as shown in Figure 2 [Chen *et al*., 1995; Wu, 1982; Kaufman and Griffiths, 1982; Wu, 1982]. The increase of possible q-values does change the energy calculation for the system, which is now described by a Hamiltonian given by [Chen *et al.*, 1995].

$$H = +J \sum_{<i,j>} \delta_{s_i,s_j} \qquad (2)$$

$$s_{i/j} \equiv spin\ values \quad : \quad \delta \equiv Kronecker\ delta\ function \ : \ J \equiv Exchange\ Energy$$
$$: H \equiv Hamiltonian\ Energy\ Value$$

This equation will have either a $+J$ or a $-J$ depending on whether it is describing a ferromagnetic or antiferromagnetic Potts model, respectively. The general Hamiltonian calculation comes from classical mechanics and is defined as the total energy. This general equation contains kinetic energy, but in this case the kinetic energy is not considered.

1.1.3 Antiferromagnetic Potts Model:

Initially, the Antiferromagnetic Potts model lacked rigorous research because of the issues involved with the simulation process [Wu, 1982]. A significant difficulty that researchers faced was extremely long relaxation periods at low temperatures near critical behavior [Wang *et al.*, 1989]. The ability to more deeply research this field has been aided by the work of both Robert Swendsen and Jian-Sheng Wang through the development of the Swendsen-Wang cluster flip algorithm [Wang *et al.*, 1989, Chen *et al.*, 1995]. This cluster flip algorithm drastically reduces the relaxation time by taking a different statistical approach than a single flip algorithm. Both of these authors have contributed more than just this specific algorithm needed for this instance, but it has proven to be one of the pivotal algorithms for simulating the Antiferromagnetic Potts model at all temperatures.

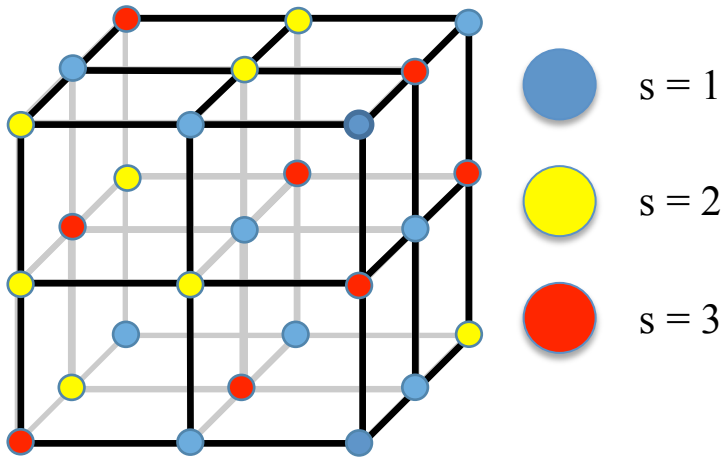


Figure 2: Diagrammatic representation of a 3-dimensional Potts model. This model has a q-value of 3, which means that each element has 3 possible orientations (of spins). The three colors correspond to the three possible orientations. Alternatively, the system can be thought as made of three different types of atoms.

1.2 Research on Applications of the Models:

The typical lattice considered for the Potts and Ising models is an ideal lattice. This means a lattice with uniform bonds and atomic structures. However, real world systems do not have ideal structures, even at temperatures of absolute zero. This makes the effects of defects an area of interest and there has been research done for both the Ising and Potts models. Most research on defects is focused on the effect on the critical behavior. The research of Kaufman and Griffiths (1982) and Chen *et al.* (1995) on the critical temperature of phase transitions, for the Potts model, is an example of this. Blackman and Poulter (1984) and Harris (1974) have also done research on the specific heat and critical temperature of phase transitions, for the Ising model.

2 Research:

2.1 Defects:

There are several types of defects that can occur within a lattice. Some examples of these defects are line, ladder, diagonal, planar, and point [Christensen, 2000; Kaufman and Griffiths, 1982]. The point defect is the simplest of these defects and so it seems to be a natural starting place. The point defect can occur in four different ways as shown in Figure 3 [Christensen, 2000]. There can be an extra atom inside of the lattice, and this causes irregularly large gaps along the relevant lattice lines. The reverse of this is also possible if there is a missing atom causing irregularly small spaces in the relevant lattice lines. Another option is that the lattice has the correct number of indices, or atoms, but one is anomalous to the group. Lastly, an atom could not only be different to the group, but also be an unnecessary, or extra, atom. Relative to the other kinds of defects, a point defect would have the least effect on a system.

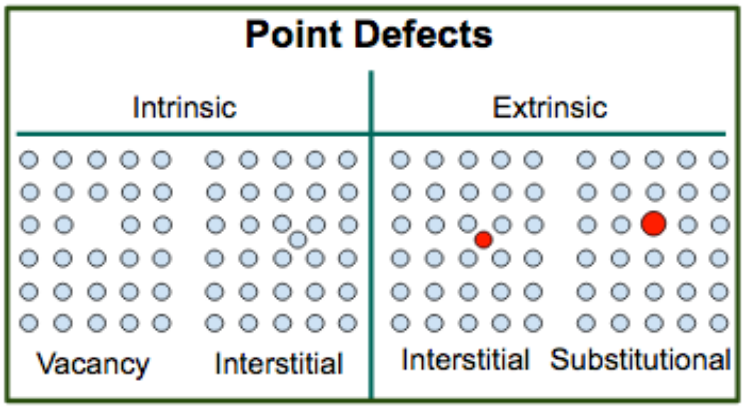


Figure 3: Diagram to show the four possible types of point defects. *Intrinsic vacancy* is a missing element in the lattice. *Intrinsic Interstitial* is an extra element of the same type inside the lattice, but at an intermediate space where no atoms are normally present. *Extrinsic substitutional* is an element of different type inside of the lattice, but at an intermediate space where no atoms are normally present. *Extrinsic interstitial* is an extra element of a *different type* at a normal lattice position.

A line defect, shown in Figure 4(a), is quite simply a line of point defects occurring along an entire row of atoms in the lattice structure [Christensen, 2000]. This can either be an extra row of atoms in the lattice, or one of the lattice's original rows can be filled with irregular atoms. When the defect runs orthogonally across the

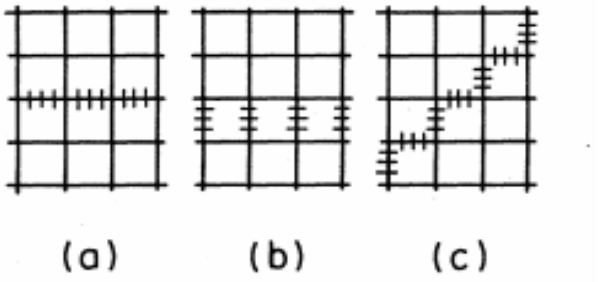


Figure 4: Lattice points occur at the intersections of the long lines, while the lines between the lattice points symbolize bonds. The lines with short hair-like lines perpendicular to them indicate defects: (a) a line defect, (b) a simple ladder defect, (c) a diagonal defect. [Kaufman and Griffiths, 1982]

bonds in the lattice, it is called a ladder defect, shown in Figure 4(b). This defect is not due to a clumping of point defects, but rather occurs due to the lattice bonding improperly while it forms. The ladder defect is related to the planar defect. In essence, the planar defect is a three-dimensional case of the ladder defect, which means that there is an entire two-dimensional plane inside of the three dimensional cube with defective bonds. Imagine two lattice faces next to each other; however, instead of being parallel to one another they form a slight angle between the two. This irregular distance causes the defective bonds. Diagonal defects also occur due to improper lattice bonding. It can be viewed more clearly in Figure 4(c), but can be visualized as each bond defect being connected at ninety degrees to the previous. The diagonal defect is specific to a two dimensional lattice.

2.1.1 Effect of Defects:

The concept of defects in the Ising and Potts models is not overly complex. The focus is to generate randomly distributed bond defects throughout the simulated model before the Markov Chain Monte Carlo runs. These bonds will have differing energy values from the rest of the system. These unique energy values will effect the probability of bonds forming, flipping, and the overall energy value of the system. Analyzing the effects of these defects in the system could have applications in many areas of science. A specific example of this is doped semi-conductors. Introducing foreign atoms, or defects, into the structure can increase the conductivity of certain semi-conductors. It could be possible to use a defect-Potts model to help simulate and optimize these effects in semi-conductors [Skorupska, 2013].

2.2 Phase Transitions and Critical Behaviors:

The introduction of defects into the Potts model will have an effect on the phase transitions and critical behaviors of the system. A phase transition occurs when a region of uniform physical properties transforms due to heat transference. Paul Ehrenfest developed the initial classification of phase transitions, in 1933, based on jumps in the derivatives of the free energy function [Jaeger, 1998]. These classifications were later generalized to first-order and continuous transitions [Jaeger, 1998]. When the first order derivative of the free energy is discontinuous, the system is classified as a first order transition. When the second-order and higher derivatives are discontinuous, the system is

classified as a continuous transition. It is at these phase transitions that critical behaviors, such as transition from a magnetized to a non-magnetized (disordered) system occur. Critical behaviors are important states or functions of a system, and the presence of defects will potentially change them.

2.3 Markov Chains:

Simulating an Ising or Potts model begins with a Markov Chain. A Markov Chain is a sequence of events in which the occurrence of the next event is uniquely dependent on the most recently considered event and none of the events previous to this [Swendsen and Wang, 1987]. So each time the chain takes a step, the next step is only dependent on the previous one. The Markov Chain can be seen in many natural processes such as Brownian motion [Swendsen and Wang, 1987]. Developing scientific models that mimic natural processes is a common practice as it allows one to study the powerful patterns that occur in nature. However, the system must normalize in order to reach an invariant distribution (equilibrium) before we can collect data points from a Markov Chain. This portion of the data, before we can collect it, is known as a burn run. There is an estimator called the ergodic average that can be used to find how far into the chain the steps must go before the data becomes relevant [Gilks *et al.*, 1996].

$$\bar{f} = \frac{1}{n-m} \sum_{t=m+1}^{n} f(x_t) \qquad (3)$$

$$\bar{f} \equiv ergodic\ average$$

$$n \equiv furthest\ step \ : \ m \equiv initial\ step$$

$$x_t \equiv variable\ for\ current\ step$$

For short run lengths the estimator is required calculate how long it will take to equilibrate a system. However, for runs that are approximately one million steps or greater, as most runs commonly are, using the ergodic average is often considered to be unnecessary because it has been found that discarding the initial one to two percent of the total run length will function as an acceptable burn-length [Gilks *et al.*, 1996]. After the burn-run we begin to collect the data set, which is then used for a Monte Carlo simulation.

2.4 Monte Carlo Simulation:

Monte Carlo method is a statistical simulation used in fields ranging from finance to physics and has also found widespread use in social sciences as well as humanities. We are utilizing the strength of Monte Carlo simulation to model disorders inherent in real life systems that can be modeled by the Potts and the Ising models. This begins by using simulated data set to create a probability distribution for a given system of events [Gilks *et al.,* 1996]. Using the distribution it calculates average values and approximated expectation values that can be used to analyze a system, and potentially help find ways to optimize that system.

2.5 Metropolis Algorithm:

The Markov Chain Monte Carlo method needs a probability algorithm to decide where each of its steps heads to and what occurs at said step. Traditionally, the Metropolis Algorithm, which is classified as a spin-flip algorithm, has been used to run MCMC. This algorithm moves in a step-by-step manner and determines each configuration flip based on two probability distributions, a target distribution and a proposal distribution [Gould and Tobochnik, 1986]. The proposal distribution affects the next point of focus and the target distribution determines whether or not that configuration is flipped to a new state or left in its current state. This is a well-accepted process, but there are issues. The Metropolis Algorithm is fairly arduous, even for a computer, when working with large multi-dimensional arrays. As the temperature decreases or as the system approaches a phase transition, in the antiferromagnetic Potts model, the amount of time needed to reach two independent configurations continuously increases. This period of time is referred to as the relaxation time [Wang *et al.*]. The issue is that critical behavior occurs around low temperatures, so this increasing relaxation time is a problem. Thus, reducing the time between state flips is imperative if the calculations are to be completed in a reasonable amount of time.

2.6 Swendsen-Wang Algorithm:

The SW algorithm is particularly effective at reducing critical slowing down. It is known as a cluster-flip algorithm because instead of flipping, or not flipping, a single spin at a single time, as in the metropolis algorithm, it flips or does not flip entire clusters

within the system. The SW algorithm bonds nearest neighbor spins with a proportional probability described by [Swendsen and Wang, 1987].

$$P(J) = 1 - \exp(-2J\beta) \qquad (4)$$

$$J \equiv Bond\ energy \quad : \quad \beta \equiv \frac{1}{k_B T}$$

β is inverse temperature where k_B is the Boltzmann Constant and T is temperature. Clusters are then identified based on continuously bonded sites (sites that are continuously bonded belong to the same cluster.). These clusters are then flipped based on a probability of $\frac{1}{2}$ [Swendsen and Wang, 1987]. Figure 5 shows a helpful visualization of this cluster flipping process. This process of creating new bonds and forming clusters is repeated for every Monte Carlo Step.

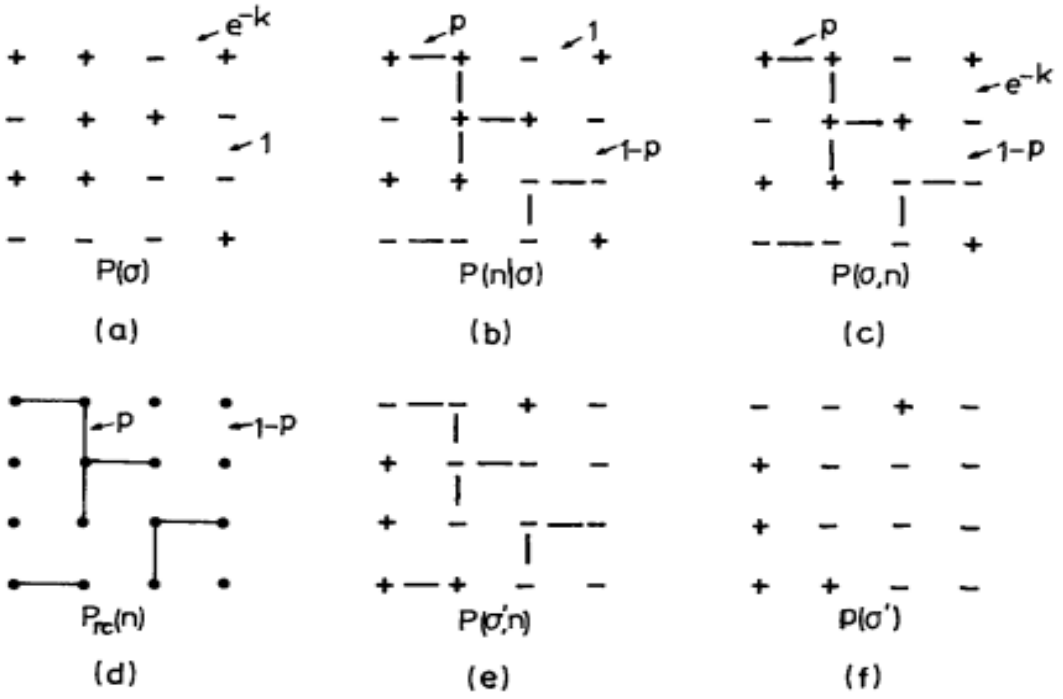


Figure 5: Diagram to show the steps of a q=2, ferromagnetic SW Monte Carlo flip. (a) a Potts state with given spins; (b) the conditional probability for sites bonding given the spins; (c) a configuration of the joint model of Potts spins and bond probabilities; (d) different clusters of value {n} where the single dots are considered clusters of one element; (e) the new flipped state for the joint model; (f) the new and final Potts state. [Wang and Swendsen, 1990].

2.6.1 Cluster Counting:

Cluster counting is a vital computational component of the Swendsen-Wang Cluster Flip. There are several algorithms that can be used to perform this counting task, but one of the more effective ones is the Hoshen-Kopelman Algorithm. This is the process of assigning a value label to each cluster as they are encountered. Bonds being formed between elements create a cluster, and not every element that has the possibility of bonding will actually bond. The algorithm ensures that each cluster is appropriate labeled or re-labeled depending on sites connected to each cluster. If a cluster is labeled with a high value and then later found to be connected to a low value cluster the algorithm must then re-label the higher value cluster to have the same value as the lower value cluster, as depicted in Figure 6. The Hoshen-Kopelman algorithm uses a technique that allows this re-labeling to be accomplished within one scan of the lattice, while other algorithms might require multiple scans to accomplish the same task. This algorithm is highly efficient in terms of computer simulation.

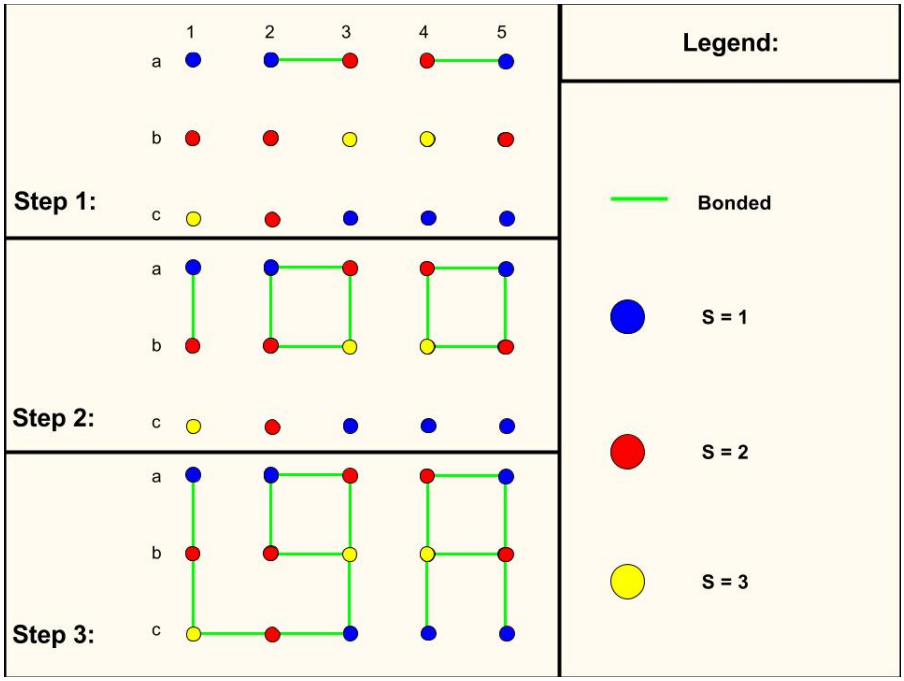


Figure 6: This depicts the first three steps for cluster counting with the Hoshen-Kopelmann algorithm in a 3x5 lattice. The count moves from row (a) downwards and each cluster is given a value of C(n+1) starting at n=0. As the count continues clusters are labeled and re-labeled in the appropriate way. In step 1 only the first row is scanned and 3 clusters are found: C(1) [a1], C(2) [a2–a3], C(3) [a4-a5]. Then step 2 considers row (b) and expands cluster labels: C(1) [a1-b1], C(2) [a2-a3-b2-b3], C(3) [a4-a5-b4-b5]. Step 3 is two fold, the initial count: C(1) [a1-b1-c1-c2-c3], C(2) [a2-a3-b2-b3-c3], C(3) [a4-a5-b4-b5-c4-c5]. The re-labeling: C(1) [a1-b1-c1-c2-c3-a2-a3-b2-b3], C(2) [a4-a5-b4-b5-c4-c5].

3 Background Theory:

3.1 Summary of Background Theories:

The Potts model is a reasonably common statistical model. It finds use in the fields of statistical mechanics, thermodynamics, electromagnetism, and classical mechanics. We use this model as our base for finding specific heat, magnetization, and Hamiltonian energies. We are investigating a classical model for this project, so I will be leaving out the model's relationship to quantum mechanics in my derivations.

3.2 Percolation Theory:

Percolation theory is one of the few theoretical techniques that are effective at dealing with severely disordered systems, such as the Potts and Ising models [Zallen, 1983]. The concept of percolation itself is the progression of a substance through a material with systems of blocked and unblocked paths. An example of this could be water running through a filter. We use percolation theory to observe the random propagation of disorder through our lattice by observing cluster connections that form during simulation. One type of percolation theory is known as site percolation, which uses discrete rather than continuous values. Site percolation focuses on the percolation from element to element rather than the percolation from path to path between the elements. Percolation theory helps to conceptually describe what Monte Carlo simulation is doing, but does not actually provide the algorithms used for simulation of these severely disordered systems.

3.3 Specific Heat:

The theory behind specific heat stems from thermodynamics due to its relationship to phase transitions. Magnetization also has a connection to order-disorder systems, but stems from electromagnetism. Electromagnetism describes magnetization because each electron has a spin, which generates a magnetic field, and when these fields are all in the same direction we wind up with a magnetic object. Specific heat is defined as the heat per spin required to raise the temperature of the spin of a given system by one unit, in our case 1 K [Gould and Tobochnik, 1986]:

$$c = \frac{C}{N} = \frac{< E^2 > - < E >^2}{T^2} \qquad (5)$$

where C is the heat capacity, *N* is the total number of elements in system, T is the temperature, $< E^2 >$ is the average squared energy, and $< E >^2$ is the average energy squared. This relationship is derived in the appendix. Heat capacity is the number of heat units required to raise the temperature of a body by one degree. This increase of temperature causes the system to move from an ordered state to a slightly more disordered state, and this is a key concept in thermodynamics. While specific heat depends conceptually on thermodynamics, we need the help of statistical mechanics to gain mathematical insight into it.

3.4 Statistical Mechanics:

Statistical mechanics helps us to handle the large number of elements included in the system. We must remember that flipping a spin is dependent on a probability distribution. To bring this dependence in, we normalize our average energy values to a partition function unique to the system:

$$Z = \sum_{\alpha} e^{-\beta E_{\alpha}} \qquad (6)$$

where Z is the partition function, and E_{α} is the energy of the considered element. The partition function is a sum of Boltzmann distributions, which deals with the probability distribution of particles in a system over various possible states. This helps us to bring all of the elements cohesively into our considered system.

3.5 Magnetization:

Magnetization does not even require a derivation. It is simply defined by the summation of the direction of the spin elements, specifically magnetic moments, in the system, which is again directly related to a move from, order to disorder or vice versa.

$$\bar{M} = \frac{\sum_i s_i}{N} \qquad (7)$$

Equation 7 is the average magnetization, where s_i is the spin orientation of the observed element and *N* is the total number of elements in the array. Specifically for the Ising model, the spin orientation can only be either up {+1} or down {-1}. So magnetization gives us the ratio of the difference between spin up and spin down elements to total number of elements, which gives us the magnetization of the system.

4 Analysis:

4.1 Summary of Methods:

I will be using Markov Chain Monte Carlo (MCMC) with a SW algorithm to generate my data. The long-term objective is to systematically introduce more and more defects into a three-dimensional Antiferromagnetic Potts model and observe changes to quantities of interest such as specific heat, magnetization, and transition temperatures. In the first semester, I worked with the two-dimensional Ising model with the purpose of familiarizing myself with computational work by doing some programming and to learn techniques used to analyze data typical in MC simulations. This semester, I worked with the three-dimensional antiferromagnetic Potts model on a cubic lattice. I wrote a subroutine to introduce defects in this system. This subroutine involves generating random lattice coordinates to identify sites, which will be converted to defects. It also required me to alter some other parts of the program so that these sites do not interact with other sites of the system. The biggest issue that I ran into was memory stack overflow, and both times it was traced back to the random number generator (RNG) in the program. The more perplexing issue of the two was that when I would attempt to generate a lattice with seventy percent or larger defects, regardless of the lattice size, the program would have a segmentation fault. At first I thought that it must be the boundary conditions within the program struggling to deal with such a large percentage of the surface having defects, but as it turned out the maximum value that I had set on the RNG was too small and seventy percent happened to be the threshold. When considering the effects of introduced defects, the outputs of the model in which defects are present must be compared against outputs of the model in which defects are not present. There should be a noted difference in where the phase transitions occur and the characteristics of the critical phenomena. Curves will be fit to different data sets such as specific heat and magnetization. This will allow for a clearer view of the discrepancies between outputs with defects and outputs without defects.

4.2 Program:

I have not yet begun working with the three-dimensional Potts model program; however, I am using a lot of the concepts that I will need by working with the two-dimensional Ising model. While the program for the Ising model can be altered easily to

run at reasonably high lattice sizes, it is fairly rudimentary and tends to have data outliers at these higher lattice values. I have found that lattice sizes below 32x32 tend to be reasonable and so this has been the range for my simulations. My program requires initial input values (i) lattice size, (ii) percentage of defects in the lattice, (iii) temperature range to be sampled, and (iv) the increment, with which to move through the temperature range. The program takes these values, equilibrates the system, and then applies MCMC. It collects the data and calculates several quantities, which can be used to analyze different properties of the system. Some of the outputs are (i) mean energy per spin, (ii) mean magnetization per spin, and (iii) specific heat per spin. Graphing these against the temperature range gives insight into critical behaviors such as the critical temperature, magnetization, and phase transitions.

4.3 Data Analysis:

Once the program produces my data I draw graphs using a program called Kaleidagraph. It allows me to tailor details of my graph to the data. The magnetization of a system can be found by graphing the mean magnetization per spin against the temperature, critical temperature of the system can be found by graphing specific heat per spin against the temperature because the specific heat undergoes a divergence at the critical temperature. These critical behaviors are then fitted with best-fit curves. I then compare the non-defect output curves to the defect output curves to determine the effects of the defects, Figures 7 and 8 display examples of these comparisons. Figure 9 displays a comparison of three different Ising lattice sizes, all without defects. This semester, I applied the knowledge from my work with the Ising model to the Potts model. For the 3-dimensional case, I have run simulations for both 8x8x8 and 64x64x64 lattices across a range of defect percentages. Even with the system scaling up to three dimensions and having a q-value of three rather than two, the data produced still follows similar trends. As the percentage of defects increases the phase transitions begin to flatten out and disappear. Figures 12, 13, and 14 display specific heat values, which demonstrate the loss of the phase transition. Figures 15, 16, and 17 also demonstrate this loss of phase transition through observation of magnetization values. Figures 10 and 11 show the comparison between the original Potts program and the new defect generating Potts program. Having two different lattice sizes helps to corroborate the effects of the defects

even as the system scales up to infinite lattice sizes. There are two notable changes in the data sets as the percentage of defects increases: the peaks of the critical temperature begin to shift towards lower temperatures, and the curves themselves begin to flatten out. At a high percentage of defects there is no longer a phase transition because the material is so impure that it does not retain its original properties. This result was not surprising because the properties that we were observing are present in a pure, single element, system.

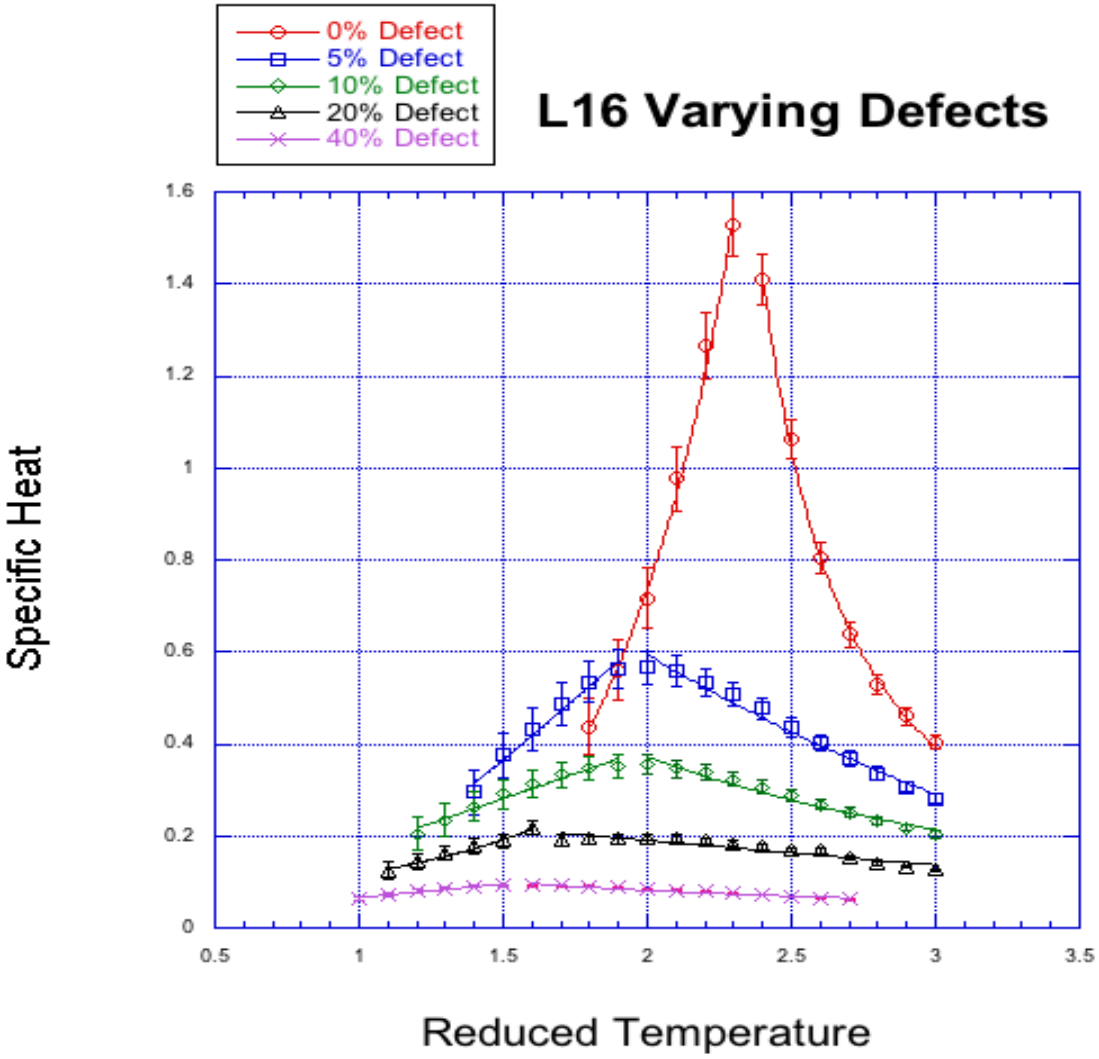


Figure 7: This is a simulation for a lattice size of 16x16. The five different curves correspond to five different levels of defects. As the percentage of defects increases the peak value of the specific heat decreases drastically and also flattens out. This indicates a loss of phase transition due to impurities.

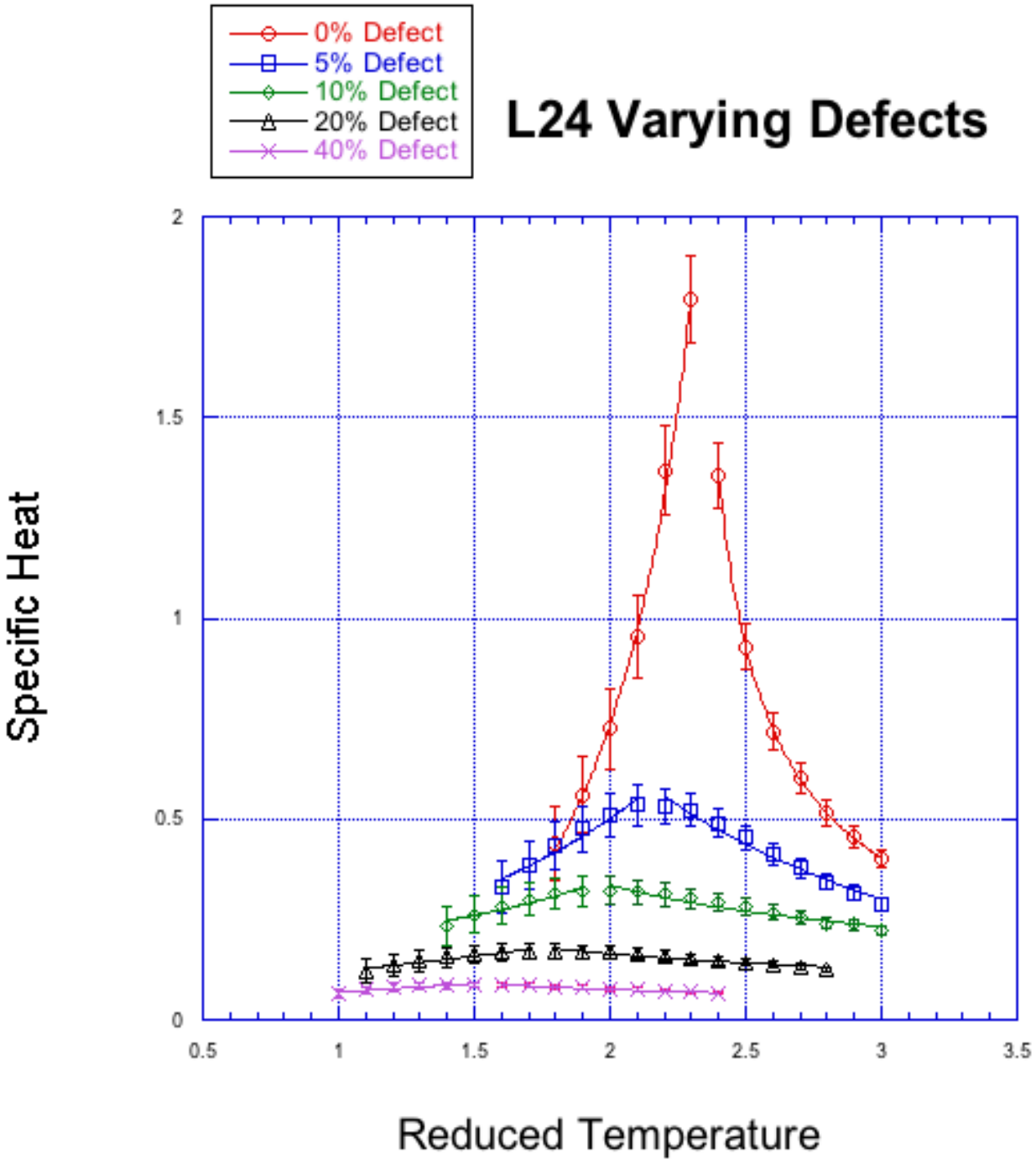


Figure 8: This is a simulation ran on a lattice size of 24x24. The five different curves correspond to five varying levels of defects introduced into the model. As the percentage of defects increases the line's peak drastically decreases which causes it to flatten. This indicates a loss of phase transition due to impurities.

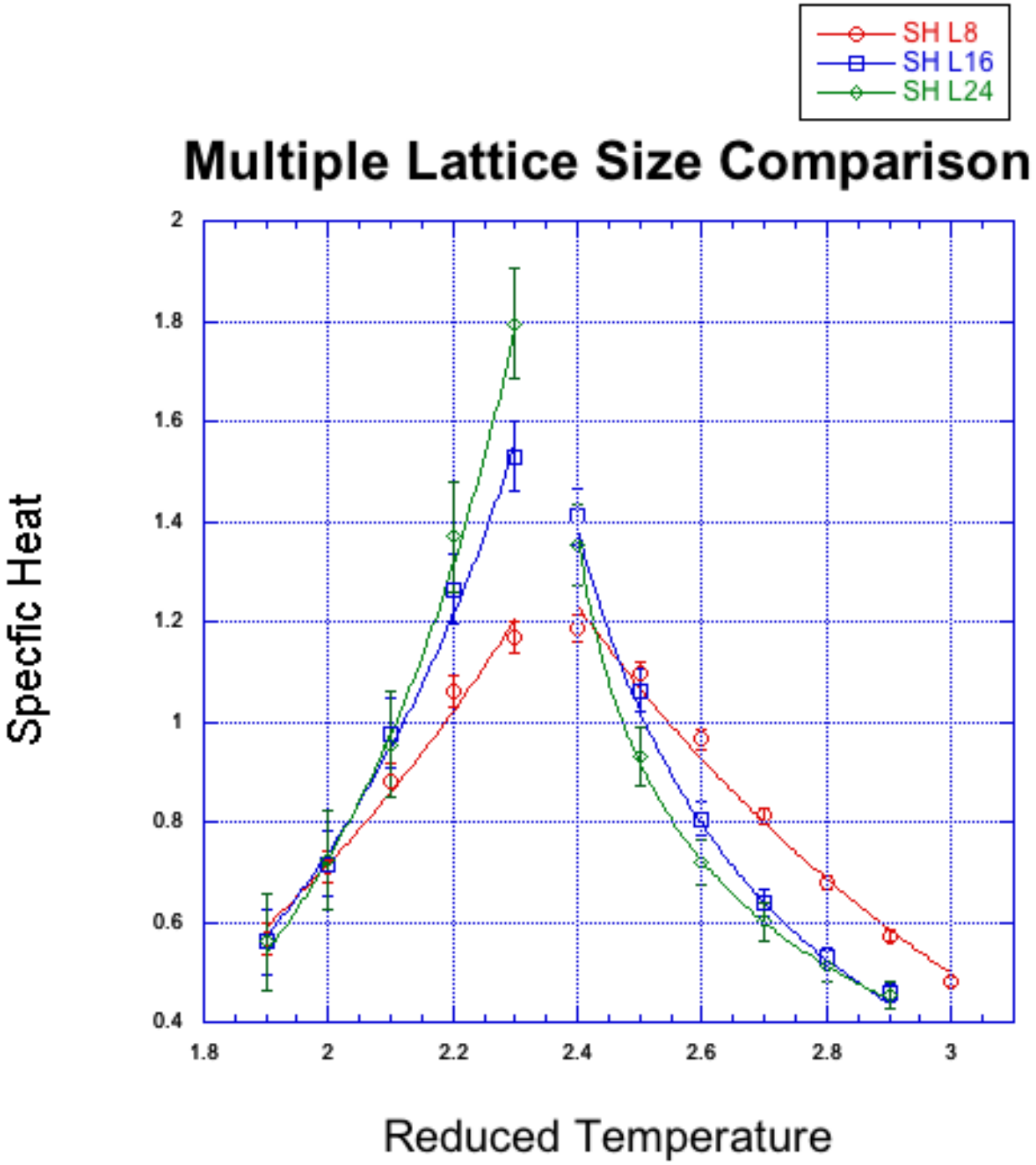


Figure 9: This figure depicts the 0% defect case for three different lattice sizes (i) 8x8 is the red data, (ii) 16x16 is the blue data, and (iii) 24x24 is the green data. As we can see as the lattice size of our system increases our specific heat values tends to approach more of a peak. This peak indicates that we are approaching a divergence in the data, which is what we expect to find in a specific heat vs reduced temperature graph. Our divergence appears to be at 2.35 Reduced Temperature. This is higher than the expected value of around 2.1.

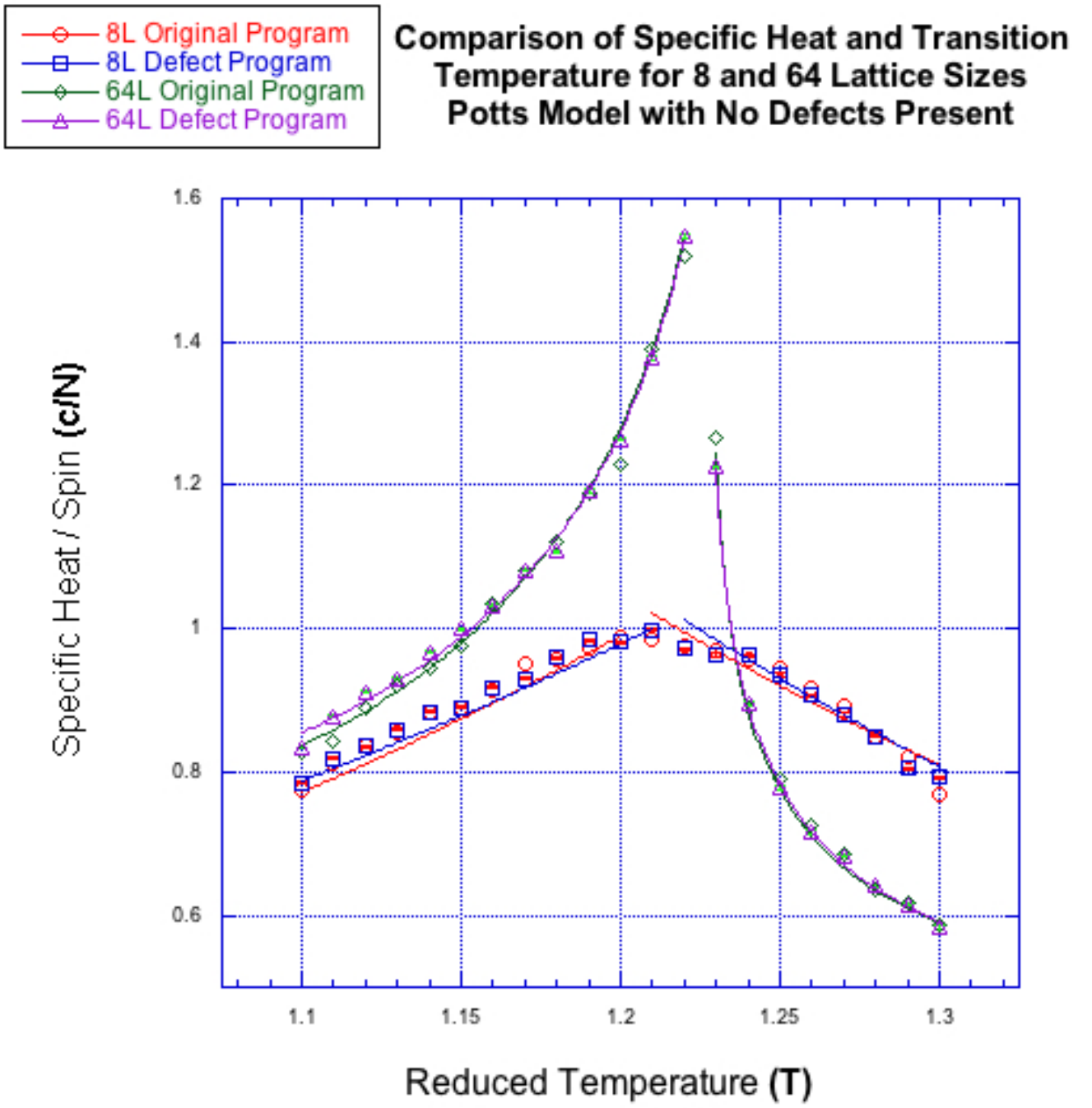


Figure 10: Comparison of both the 8x8x8 and 64x64x64 lattice data for specific heat from the defect program with no defects present and the original program. At temperature values far from the transition temperature the data is nearly identical and as the transition temperature is approached the data have slight differences. However, the trend lines indicate that the differences in specific data points are due to the statistical nature of the model.

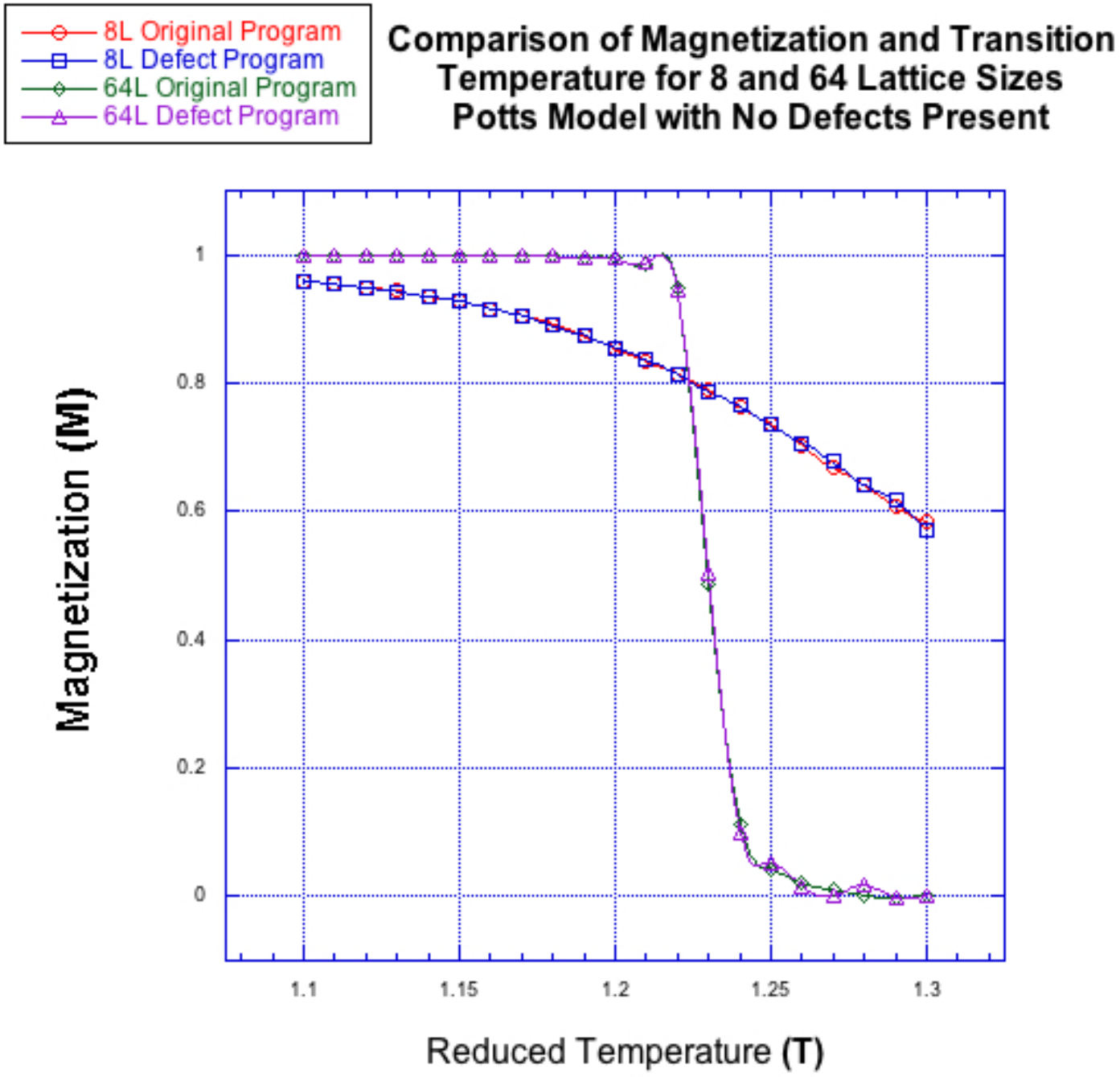


Figure 11: Comparison of the 8x8x8 and 64x64x64 lattice data for magnetization from the defect program to the original program data. These values are nearly identical which helps to confirm that the defect program is introducing defects in such a way that it is not altering the previous function of the non-defect program. The small differences in the data are from the statistical nature of the simulation and not from errors within the program.

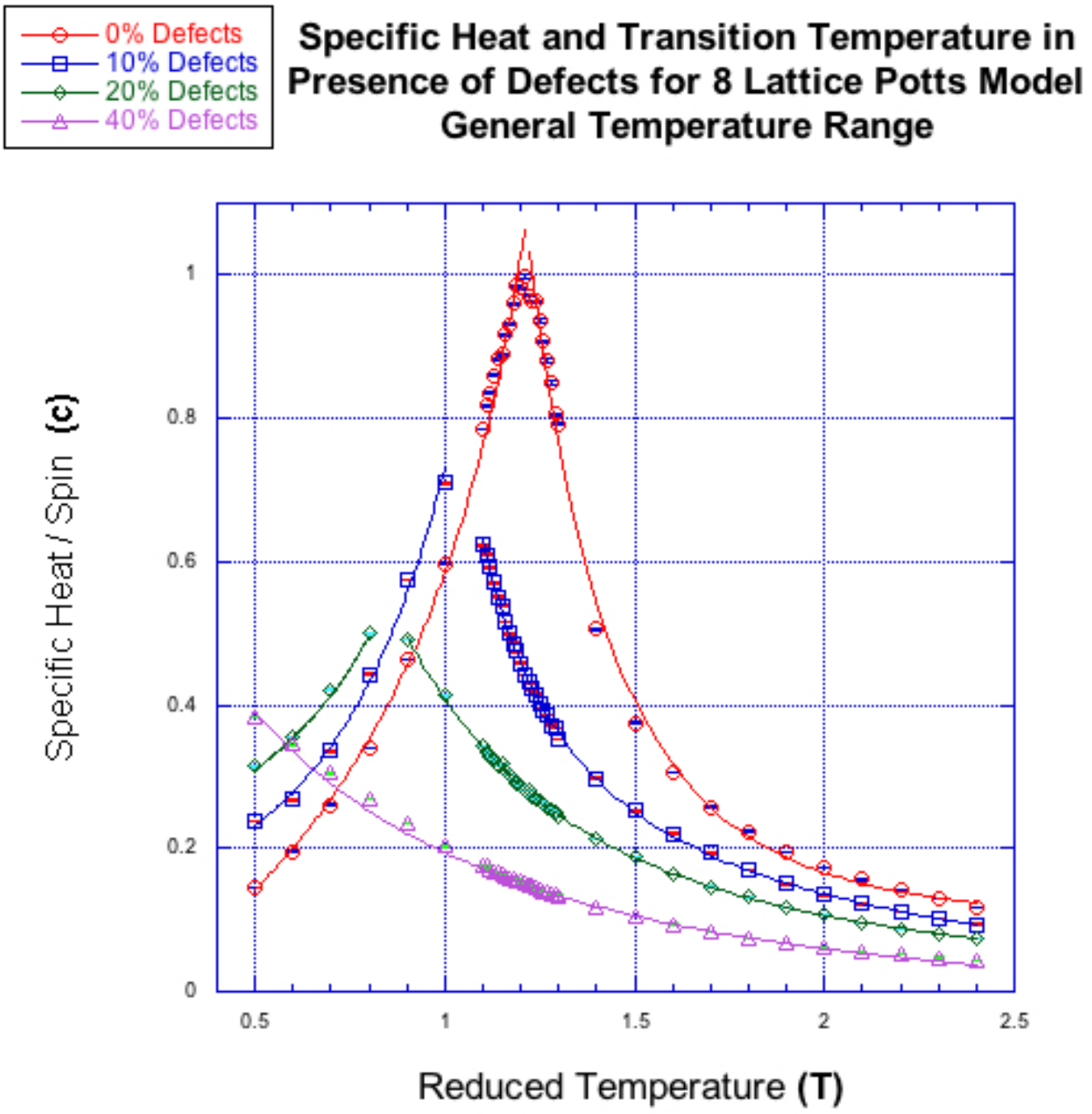


Figure 12: This graph displays the specific heat curves over the full temperature range of the 8x8x8 simulation. As the percentage of defects increases the critical temperature, which denotes the phase transition point, moves to lower temperatures and becomes less pronounced. The red curve denotes 0% defects and the critical temperature is at a value of 1.21.

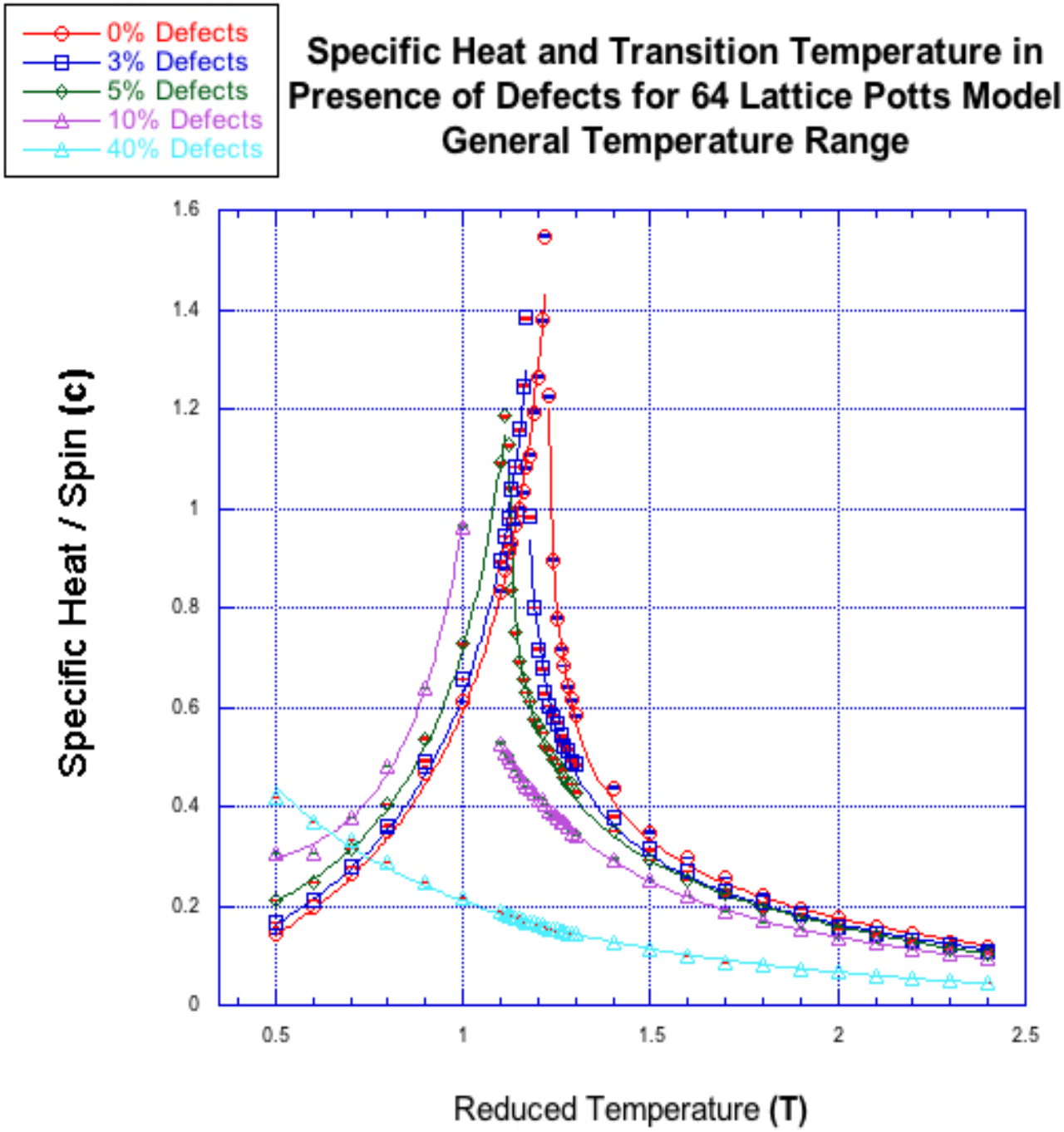


Figure 13: This is a graph of the 64x64x64 lattice simulation comparing the specific heat peaks and transition temperatures of the Potts model as the percentage value of defects is increased within the system. At low defect percentage value (the red, blue, and green data), the peaks and transition temperatures are similar but still slightly different. As the defect percentage value increases (the purple data), the peak and temperature are increasingly different from the non-defected value. At high defect percentages (the light blue data) the peak and transition temperature seems to begin to disappear.

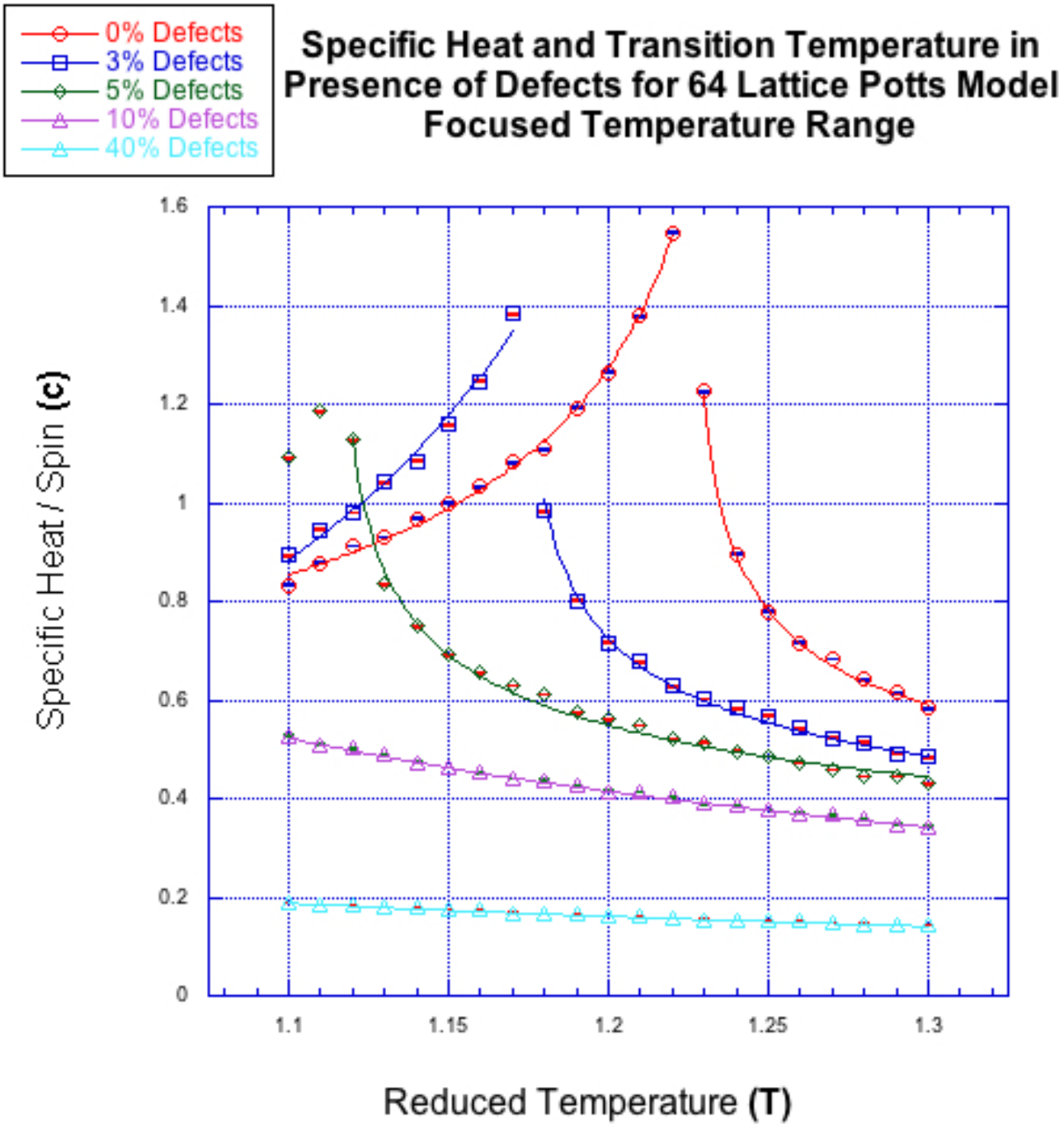


Figure 14: This is a graph of a 64x64x64 lattice focused on the range around the expected value for the 0% defect model of 1.21. The 3% and 5% defect values still have a critical temperature within the observed range, but as the defect percentage increases the critical temperature moves out of this range and the curves begin to flatten out entirely.

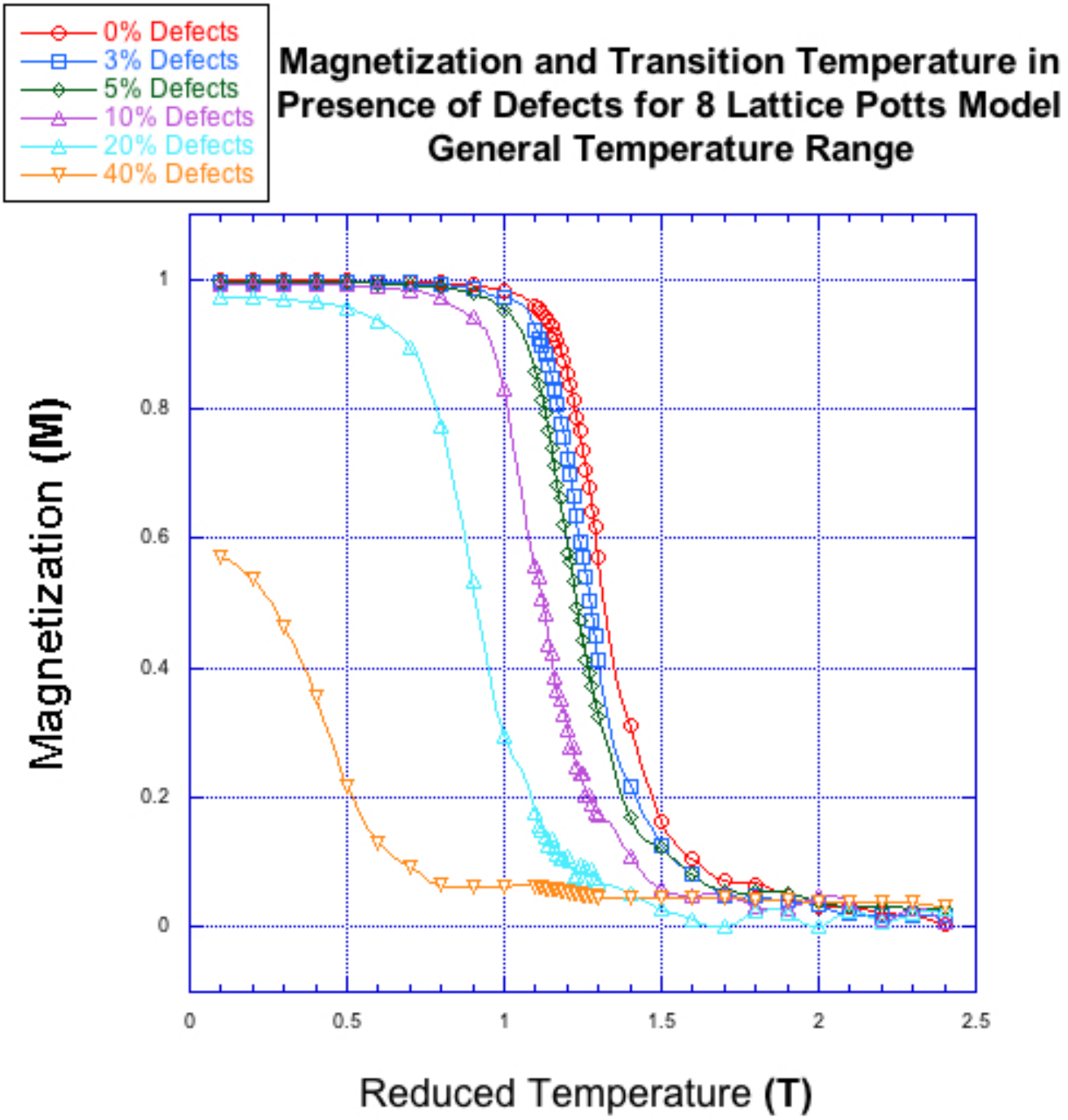


Figure 15: This is a 8x8x8 lattice graph of the magnetization of the system over the full temperature range from 0.1 to 2.4. The lower percentage defect runs do not vary drastically from the 0% defect run, but at 10% defect values there begins to be a significant change. At a value of 40% defects, the curve of the system's magnetization is significantly less than 1 in the limit of zero temperature.

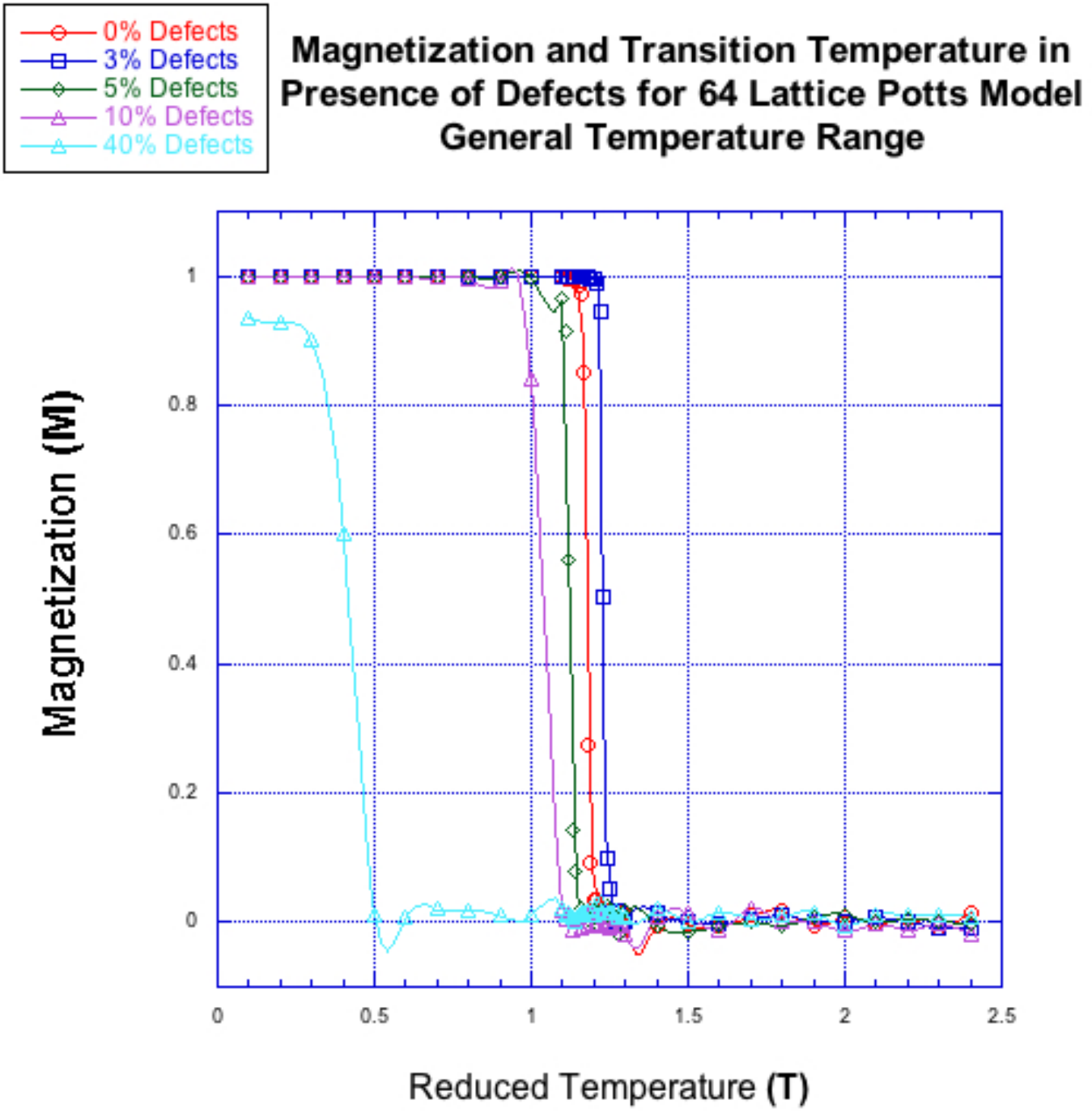


Figure 16: This is a 64x64x64 lattice graph of the magnetization of the system. At lower and even mid-range defect percentages (the blue, red, green, and purple data) the transition temperature and magnetic behavior is similar with a slight over all decrease. At high defect percentage (the light blue data) the transition temperature and magnetic behavior are much different.

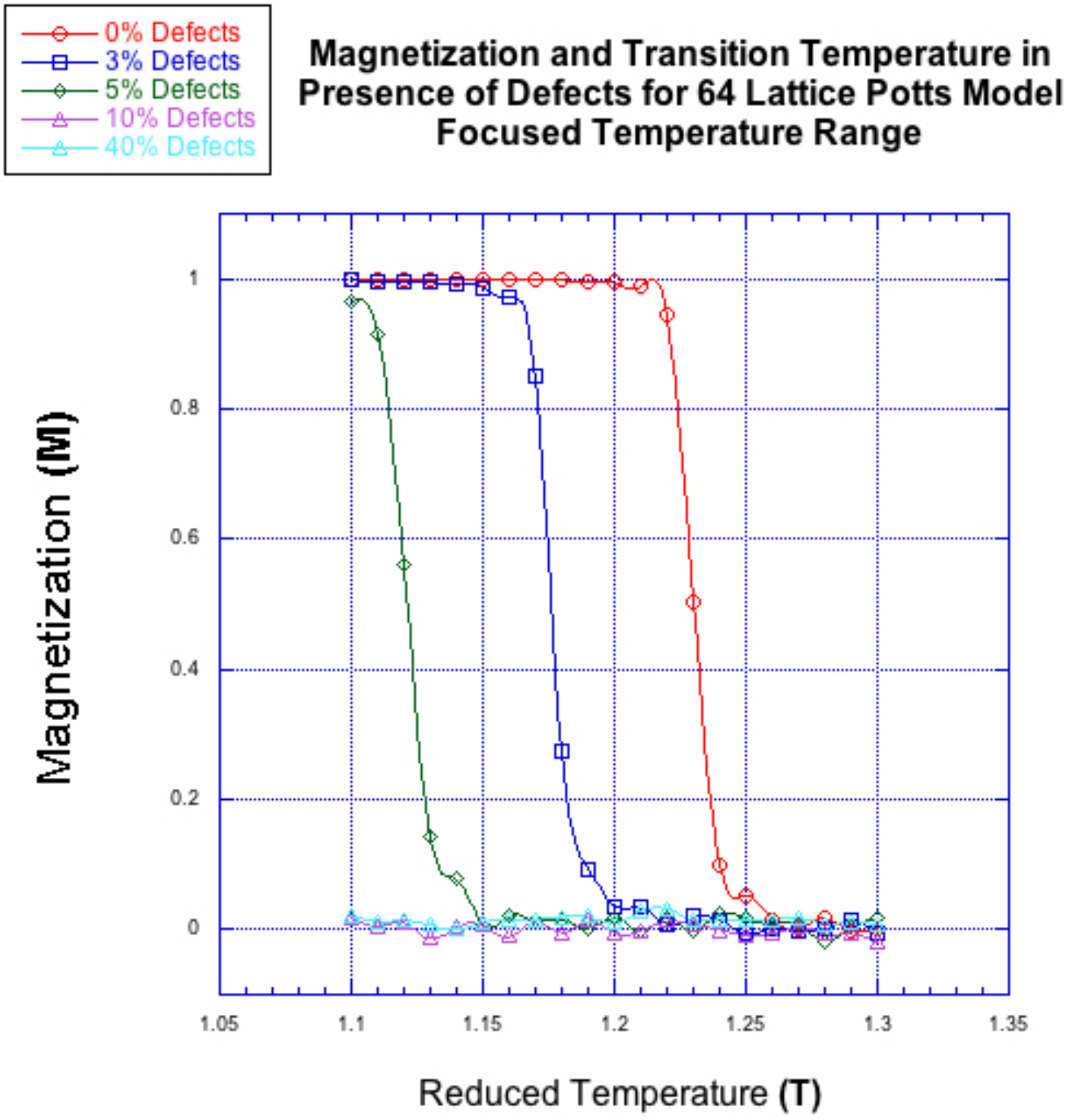


Figure 17: This is a graph of the magnetization over the focused temperature range. It more clearly displays that as the percentage of defects increases in the system the magnetization curve flattens out and the critical behavior disappears from the system.

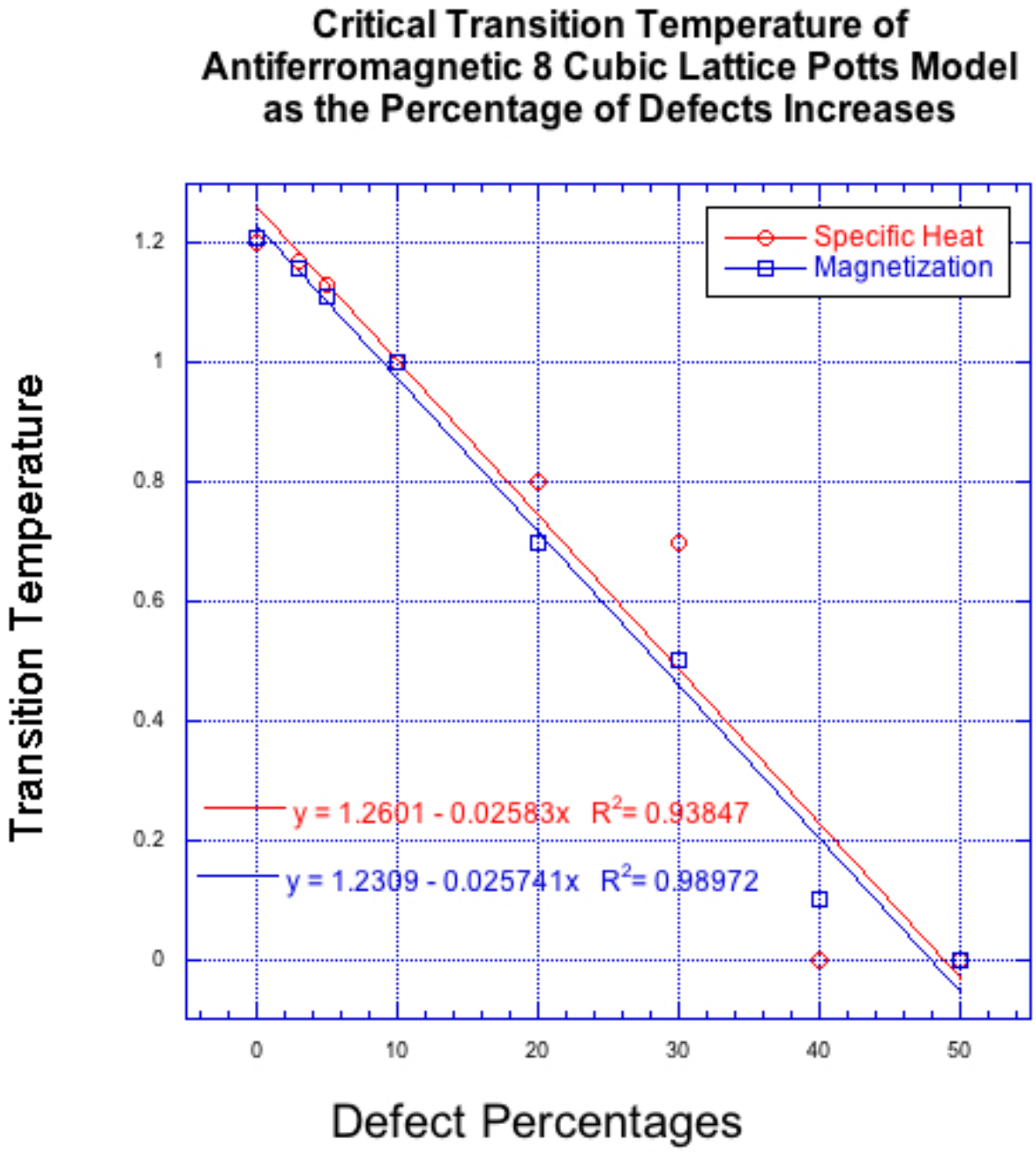


Figure 18: Depicts the decrease of the transition temperature for the 8x8x8 cubic lattice as the percentage of defects increases. These values are from both the specific heat and magnetization of the lattice and there are slight discrepancies, but the overall trend still agrees.

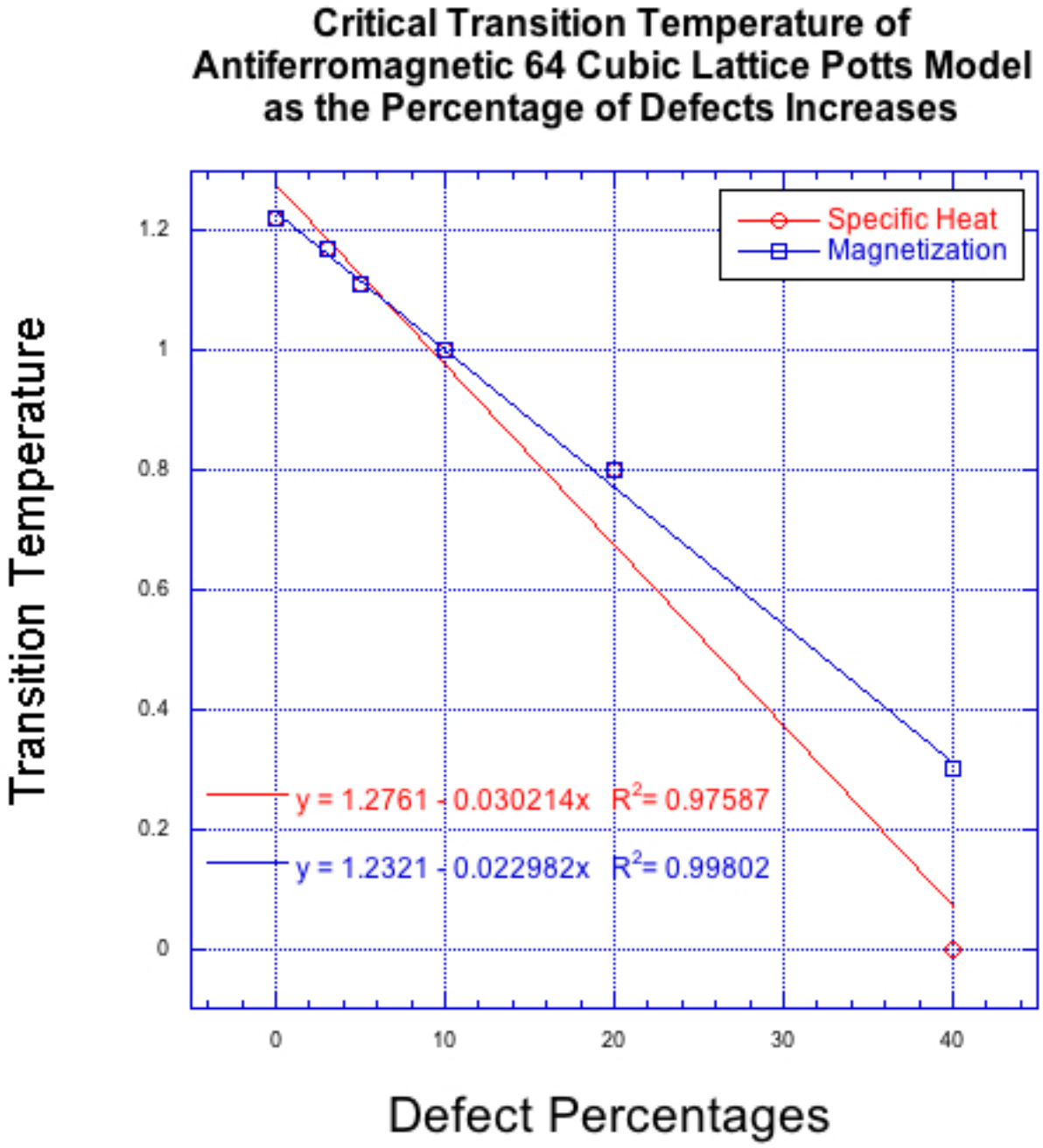


Figure 19: Depicts the values of the transition temperature for the 64x64x64 lattice as the percentage of defects increases. It is a linear trend as the defect percentage increases.

5 Conclusion:

5.1 Future Works

This project can be a conduit for a lot of future projects. One could consider defects that are foreign elements, which have interaction energies different from the original system. This adaption of the program could potentially be used to model more complex systems. However, if this route were to be taken then one would need to address some issues that exist with the random number generator. It would need to be able to generate more random values without effecting the accuracy of the outputs of the Defects Potts model. Another possibility could be using this current version of the program to observe the effects on the intermediate phase transitions. It could also be applied to fields outside of physics to be used to model different elements and observe their behaviors.

6 Acknowledgements:

Thank you to Dr. Rahman and Dr. Lombardi for the help that they gave me during this project. Also, thanks Liam.

6 Appendix:

6.1 Proof of specific heat

I will begin by defining some terms that will come up later in the derivation.
c is the specific heat while C is the heat capacity of a system. $c = \frac{C}{N}$ where N is the size of the system.
β is inverse temperature; defined as $\frac{1}{k_B T}$ where T is temperature.
U is internal energy; defined as $U = -\frac{\partial}{\partial \beta}(\ln Z) = \frac{1}{Z}\sum_i E_i e^{-\beta E_i}$.
Z is the partition function; defined as $Z = \sum_i e^{-\beta E_i}$.
There are also some simple equations from statistical mechanics that I will utilize.

$$\frac{\partial \beta}{\partial T} = \frac{-1}{k_B T^2}$$

$$\frac{\partial Z}{\partial \beta} = \sum_i E_i e^{-\beta E_i}$$

Lastly the definitions of $< E >$ and $< E^2 >$, where the summation subscript is alpha for the partition function so as not to be confused with the numerator's subscript.

$$< E > = \frac{1}{Z}\sum_i E_i e^{-\beta E_i} = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_\alpha e^{-\beta E_\alpha}}$$

$$< E^2 > = \frac{1}{Z}\sum_i {E_i}^2 e^{-\beta E_i} = \frac{\sum_i {E_i}^2 e^{-\beta E_i}}{\sum_\alpha e^{-\beta E_\alpha}}$$

Starting from the general definition of specific heat.

$$c = \frac{C}{N} = \frac{\partial U}{\partial T}$$

We can re-write the partial derivative and plug in $\frac{\partial \beta}{\partial T}$,

$$\frac{\partial U}{\partial T} = \frac{\partial \beta}{\partial T}\frac{\partial U}{\partial \beta} = -\frac{1}{k_B T^2}\frac{\partial U}{\partial \beta}$$

From here we need to evaluate the partial derivative in the definition of U and then $\frac{\partial U}{\partial \beta}$,

$$\frac{\partial U}{\partial \beta} = \frac{\partial}{\partial \beta}\left(-\frac{\partial}{\partial \beta}(\ln Z)\right) = \frac{\partial}{\partial \beta}\left(\frac{1}{Z}\sum_i E_i e^{-\beta E_i}\right)$$

$$= \left[\left(\frac{1}{Z}\sum_i E_i e^{-\beta E_i}\right)^2 - \left(\frac{1}{Z}\sum_i {E_i}^2 e^{-\beta E_i}\right)\right]$$

Plugging this solution back into our full equation we see,

$$\frac{\partial U}{\partial T} = -\frac{1}{k_B T^2}\left[\left(\frac{1}{Z}\sum_i E_i e^{-\beta E_i}\right)^2 - \left(\frac{1}{Z}\sum_i {E_i}^2 e^{-\beta E_i}\right)\right]$$

Given how we have defined our values for $< E >$ and $< E^2 >$ we get to the equation in our program.

$$c = -\frac{1}{k_B T^2}(< E >^2 - < E^2 >) = \frac{< E^2 > - < E >^2}{k_B T^2}$$

6.2 Bibliography

Blackman, J. A.; Poulter, J. "Critical Specific Heat of 2D Ising Model in Presence of Bond Defects." *J. Phys. C* **17**.1 (1984): 107-26.

Chen, S.; Ferrenberg, Alan M.; Landau, D.P. "Monte Carlo Simulation of Phase Transitions in a Two-Dimensional Random-Bond Potts Model." *Phys. Rev. E* **52**.2 (1995): 1377-86.

Christensen, Thomas M. "Structure of Solids: Defects in Solids." Physics of Thin Films. UCCS. Phys. 549. Ch. 1, Sec. 1.3. (2000). http://www.uccs.edu/~tchriste/courses/PHYS549/549lectures/defects.html Accessed: September, 2016.

Domany, Eytan; Schick, M.; Walker, J.S. "Classification of Order-Disorder Transitions in Common Adsorbed Systems: Realization of the Four-State Potts Model ." *Phys. Rev. Let.* **38**.20 (1977): 1148-51.

Ellis-Monaghan, Jo. "A gentle introduction to the Potts model."SMC. (2006). http://academics.smcvt.edu/jellis-monaghan/Talks/Intro%20to%20Potts.pdf .Web.Accessed: September, 2016.

Fitzpatrick, Richard. "The Ising Model." Computational Physics. UT. (2006). http://farside.ph.utexas.edu/teaching/329/lectures/node110.html . Web Accessed: September, 2016

Gilks, W. R.; Richardson, S.; Spiegelhalter D.J. "Introducing Markov Chain Monte Carlo." *Markov Chain Monte Carlo in Practice.* Eds. W. R. Gilks, S. Richardson, and D. J. Spiegelhalter. First ed. London: Chapman&Hall, 1996. 4-16.

Gould H and Tobochnik J. "Monte Carlo Simulation of the Canonical Ensemble. In: Introduction to computer simulation methods." First ed. Boston, MA. Addison-Wesley. 1986. Ch. 17. 565-625.

Harris, A. Brooks. "Effect of Random Defects on the Critical Behaviour of Ising Models." *J. Phys. C* **7**.9 (1974): 1671-92.

Jaeger, Greg. "The Ehrenfest Classification of Phase Transitions: Introduction and Evolution." *Archive for History of Exact Sciences* **53**.1 (1998): 51-81.

Kaufman, Miron; Griffiths, Robert B. "First-Order Transitions in Defect Structures at a Second-Order Critical Point for the Potts Model on Hierarchical Lattices." *Phys. Rev. B* **26**.9 (1982).

Kennedy, Tom “The Ising Model.” Introduction to Mathematical Physics. University of Arizona. Math. 541. Ch. 1 (2008).http://math.arizona.edu/~tgk/541/chap1.pdf Accessed: November 11, 2016.

Skorupska, Katarzyna. “Doped Semiconductors.” UWYO. (2013). http://www.uwyo.edu/cpac/_files/docs/kasia_lectures/2-intrinsicanddopedsemiconductors.pdf .Web accessed: September, 2016.

Somorjai, G. A. "Low Energy Electron Diffraction and Auger Electron Spectroscopy Studies of the Structure of Adsorbed Gasses on Solid Surfaces." *Surf. Sci.* **34**.1 (1973): 156-76.

Swendsen, Robert; Wang, Jian-Sheng. “Non-universal critical dynamics in Monte Carlo simulations.” In: *Phys. Rev.* **58** (1987): 86-88.

Wang, Jian-Sheng; Swendsen, Robert; Kotecky, Roman. "Antiferromagnetic Potts Models." *Phys. Rev. Let.* **63**.2 (1989): 109-12.

Wang, Jiang-Shen, and Swendsen, Robert H. "Cluster Monte Carlo Algorithms." *Physica A* **167** (1990): 565-79.

Wu, F. Y. "The Potts Model." *Rev. Mod. Phys.* **54**.1 (1982): 235-68.

Zallen R. The Percolation Model. In: “The Physics of Amorphous Solids.” 1st ed. Federal Republic of Germany: John Wiley & Sons Inc. (1983): 135-45

Zheng, Huaixiu; Dua, Arpit; Jiang, Liang. "Demonstrating Non-Abelian Statistics of Majorana Fermions using Twist Defects." *Phys. Rev. B* **92**.24 (2015).