We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

4,800
Open access books available

122,000
International authors and editors

135M
Downloads

Our authors are among the

154
Countries delivered to

TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities

CLARIVATE ANALYTICS
BOOK CITATION INDEX
INDEXED

WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com

Cellular Automata Simulation of Two-Layer Ising and Potts Models

Mehrdad Ghaemi
Tarbiat MoallemUniversity
Iran

1. Introduction

One of the most interesting phenomena in the physics of the solid state is ferromagnetism. Ferromagnetism and antiferromagnetism are based on variations of the exchange interaction, which is a consequence of the Pauli principle and the Coulomb interaction. In the simplest case of the exchange interaction of two electrons, two atoms or two molecules with the spins σ_1 and σ_2, the interaction has the form $E = -J\sigma_1\sigma_2$, where J is a coupling constant which depends on the distance between the spins. When the coupling constant is positive, then a parallel spin orientation is favored. This leads in a solid to ferromagnetism. This happens, however, only when the temperature is lower than a characteristic temperature known as the Curie temperature. Above the Curie temperature the spins are oriented at random, producing no net magnetic field (Fig. 1). As the Curie temperature is approached from both sides the specific heat of the metal approaches infinity.
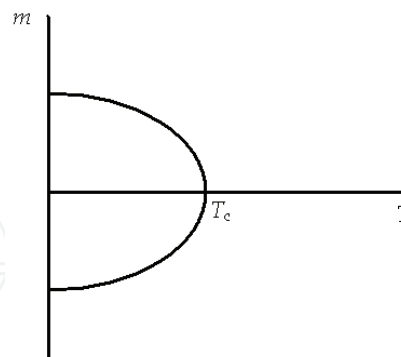

Fig. 1. Temperature dependence of magnetization

When the coupling constant is negative, then an antiparallel spin orientation is preferred. In a suitable lattice structure, this can lead to an antiferromagnetic state. The exchange interaction is short-ranged; but owing to its electrostatic origin it is in general considerably stronger than the dipole-dipole interaction. Examples of ferromagnetic materials are Fe, Ni, EuO; and typical antiferromagnetic materials are MnF2 and RbMnF3.

The Ising model is a crude attempt to simulate the structure of a physical ferromagnetic substance. This model plays a very special role in statistical mechanics and generates the

simplest nontrivial example of a system undergoing phase transitions. Its analysis has provided us with deep insights into the general nature of phase transitions which are certainly better understood nowadays after the publication of the hundreds of papers which followed the pioneering work of Onsager (Onsager, 1944).

Although, at zero magnetic field, there is an exact solution for the 2-dimensional (2-D) Ising model (Onsager, 1944 and Huang, 1984), however, there is no such a solution for the two-layer Ising and Potts models. The Potts models are the general extension of the Ising model with q-state spin lattice i.e., the Potts model with $q = 2$ is equivalent to the Ising model. Although we do not know the exact solution of the two-dimensional Potts model at present time, a large amount of the numerical information has been accumulated for the critical properties of the various Potts models. For further information, see the excellent review written by Wu (Wu, 1982) or the references given by him.

The two-layer Ising model, as a simple generalization of the 2-D Ising model has of long been studied (Ballentine, 1964; Allan, 1970; Binder, 1974; and Oitmaa & Enting, 1975). The two-layer Ising model as a simple model for the magnetic ultra-thin film has various possible applications to real physical materials. For example, it has been found that capping PtCo in TbFeCo to form a two-layer structure has applicable features, for instance, raising the Curie temperature and reducing the switching fields for magneto optical disks (Shimazaki et al., 1992). The Cobalt films grown on a Cu (100) crystal have highly anisotropic magnetization (Oepen et al., 1990) and could be viewed as layered Ising models. From the theoretical viewpoint, the two-layer Ising model as an intermediate between 2-D and 3-D Ising models, is important for the investigation of crossover from the 2-D Ising model to the 3-D Ising model. In particular, it has been argued that the critical point of the latter could be found from the spectrum of the 2-layer Ising model (Wosiek, 1994). In recent years, some approximation methods have been applied to this model (Angelini et al., 1995; Horiguchi et al., 1996; Angelini et al., 1997 and Lipowski & Suzuki, 1998). It is also argued that the two-layer Ising model is in the same universality class as the two dimensional Ising model (Li et al., 2001).

Since the exact solution of the Ising model exists only for the one- and two-dimensional models, the simulation and numerical methods may be used to obtain the critical data for other models. One of the numerical methods is using the transfer matrix and decreasing the matrix size (Ghaemi et al., 2004). Ghaemi et al. have used the transfer matrix method to construct the critical curve for a symmetric two-layer Ising model. In another work (Ghaemi et al., 2003), they have used this method to get the critical temperature for the anisotropic two-layer Ising model. Such calculations are limited to lattice with the width 5 cells in each layer and the critical point is obtained by the extrapolation approach. There are other numerical methods for solving the Ising models.

However, the numerical methods mentioned above are time consuming and advanced mathematics is required when they may be used for extended models like the anisotropic two-layer Potts model. In most cases, simulation methods are simple and fast. They are also less restricted to the lattice sizes. There are different simulation methods which have been used to describe Ising and Potts models. Monte Carlo is one of the simulation methods which has been widely used for studying Ising models (Zheng, 1998). In addition, the multicanonical Monte Carlo studies on Ising and Potts models are highly used in recent years (Janke, 1998 and Hilfer et al., 2003). The Cellular Automata (CA) are one of methods that could be used to describe the Ising model. The CA are discrete dynamic systems with simple evolution rules that have been proposed as an efficient alternative for the simulation

of some physical systems. There are some different approaches which are based on the CA method. The Q2R automaton is an approach which is used for the microcanonical Ising model. It is deterministic, reversible and nonergodic and also very fast method. Many works have been performed based on this model (Stauffer, 2000; Kremer & Wolf, 1992; Moukarzel & Parga, 1989; Stauffer, 1997; Glotzer & Stauffer, 1990; Zabolitzky & Herrmann, 1988; and MacIsaac, 1990). Although the Q2R model is deterministic and hence is fast, it was demonstrated that the probabilistic model of the CA like Metropolis algorithm (Metropolis et al., 1953) is more realistic for description of the Ising model even though the random number generation makes it slower. There is a main different between the Cellular Automata (CA) method and the Monte-Carlo method which is in the updating of a system in each step. In the Monte-Carlo method, only one site or a cluster which is randomly chosen is updated in each step. However, in the CA, all sites are updated in each time step without a random selection.In addition to the Monte Carlo method, it was proposed that the Cellular Automata (CA) could be a good candidate to simulate the Ising models (Domany & Kinzel , 1984).

In the last two decade a large amount of works were done for describing Ising models by the CA approach and a great number of papers and excellent reviews were published (MacIsaac, 1990; Creutz, 1986; Toffoli & Margolus, 1990; Kinzel, 1985; and Aktekin, 1999). Most of the works that have been done until now are focused on the qualitative description of various Ising and Potts models or to introduce a faster algorithm. For example, the Q2R automaton as a fast algorithm was suggested which has been studied extensively (Vichniac, 1984; Pomeau, 1984; Herrmann, 1986; Glotzer et al., 1990; Moukarzel & Parga, 1989; and Jan, 1990). It was so fast, because no random numbers must be generated at each step. But in the probabilistic CA, like Metropolis algorithm, generation of the random number causes to reduce the speed of calculation, even though it is more realistic for describing the Ising model.

2. Isotropic two-layer Ising model

Consider a two-layer square lattice with the periodic boundary condition, each layer with r rows and p columns. Each layer has then $r \times p$ sites and the number of the sites in the lattice is $2 \times r \times p = N$. We consider the next nearest neighbor interactions as well, so the number of neighbor for each site is 5. In the two-layer Ising model, for any site we define a spin variable $\sigma^{1(2)}(i,j) = \pm 1$ in such a way that $i = 1,...,r$ and $j = 1,...,p$ where superscript 1(2) denotes the layer number. We include the periodic boundary condition as

$$\sigma^{1(2)}(i+r,j) = \sigma^{1(2)}(i,j) \tag{1}$$

$$\sigma^{1(2)}(i,j+p) = \sigma^{1(2)}(i,j) \tag{2}$$

The configuration energy for this model may be defined (Ghaemi et al., 2003) as:

$$\frac{E(\sigma)}{kT} = -\sum_{i=1}^{r,*}\sum_{j=1}^{p,*}\sum_{n=1}^{2}\{K_x\sigma^n(i,j)\sigma^n(i+1,j)+$$

$$K_y\sigma^n(i,j)\sigma^n(i,j+1)\} - K_z\sum_{i=1}^{r}\sum_{j=1}^{p}\sigma^1(i,j)\sigma^2(i,j) \tag{3}$$

where * indicates the periodic boundary conditions (eqs 1,2), and Kx and Ky are the nearest-neighbor interactions within each layer in the x and y directions, respectively, and Kz is the interlayer coupling.

Therefore, the configuration energy per spin is

$$e = \frac{E(\sigma)}{kTN} \tag{4}$$

The average magnetization of the lattice for this model can be defined (Newman & Barkema, 2001) as

$$\langle M \rangle = \left\langle \sum_{i=1}^{r,*} \sum_{j=1}^{p,*} \sum_{n=1}^{2} \sigma^n(i,j) \right\rangle \tag{5}$$

and the average magnetization per spin is

$$\langle m \rangle = \frac{\langle M \rangle}{N} \tag{6}$$

The magnetic susceptibility per spin (χ) and specific heat per spin (C) is defined as

$$\frac{\partial < M >}{\partial \beta} = \beta(< M^2 > - < M >^2) \tag{7}$$

$$\chi = \frac{\beta}{N}\left(\langle M^2 \rangle - \langle M \rangle^2\right) = \beta N \left(\langle m^2 \rangle - \langle m \rangle^2\right) \tag{8}$$

$$C = \frac{k\beta^2}{N}\left(\langle E^2 \rangle - \langle E \rangle^2\right) = k\beta^2 N \left(\langle e^2 \rangle - \langle e \rangle^2\right) \tag{9}$$

where $\beta = \frac{1}{kT}$.

In the present work, we considered the isotropic ferromagnetic and symmetric case i.e. $K_x = K_y = K_z = K \geq 0$. We have used a two-layer square lattice with 2500×2500 sites in each layer with the periodic boundary condition. The Glauber method (Glauber, 1963) was used with checkerboard approach to update sites. For this purpose the surfaces of two layers are checkered same as each others. For updating the lattice, we use following procedure: after updating the first layer, the second layer could be updated.

The updating of the spins is based on the probabilistic rules. The probability that the spin of one site will be up (p_i^+) is calculated from

$$p_i^+ = \frac{e^{-\beta E_i^+}}{e^{-\beta E_i^+} + e^{-\beta E_i^-}} \tag{10}$$

where

$$\begin{aligned} E_i^{\pm} = -K\{ &\sigma^n(i,j)\sigma^n(i+1,j) + \sigma^n(i,j)\sigma^n(i-1,j) + \sigma^n(i,j)\sigma^n(i,j+1) \\ &+ \sigma^n(i,j)\sigma^n(i,j-1) + \sigma^n(i,j)\sigma^{n'}(i,j)\} \end{aligned} \tag{11}$$

and

$$\sigma^n(i,j) = +1 \text{ for } E_i^+$$
$$\sigma^n(i,j) = -1 \text{ for } E_i^-$$

(12)

and $\sigma^{n'}(i,j)$ is the neighboring site (i,j) in the other layer. Hence, the probability that the spin to be down is

$$p_i^- = 1 - p_i^+$$

(13)

The approach is as follow: first a random number is generated. If it is less than p_i^+, the spin of the site (i,j) is up, otherwise (it means that random number is greater than p_i^+), it will be down.

When we start CA with the homogeneous initial state (namely, all sites have spin up or +1), before the critical point (K_C), the magnetization per spin (m) will decay rapidly to zero and fluctuate around it. After the critical point, m will approach to a nonzero point and fluctuate around it; and with increasing of K, the magnetization per spin will increase. But at the critical point, m will decay very slowly to the zero point and the fluctuation of the system will reach to a maximum. For each K, the time that m reaches to the special point and starts to fluctuate around it is called the relaxation time (τ). On the other words, the relaxation time is the time that the system is thermalized. The value of τ can be obtained from the graph of m vs. t (Fig. 2).

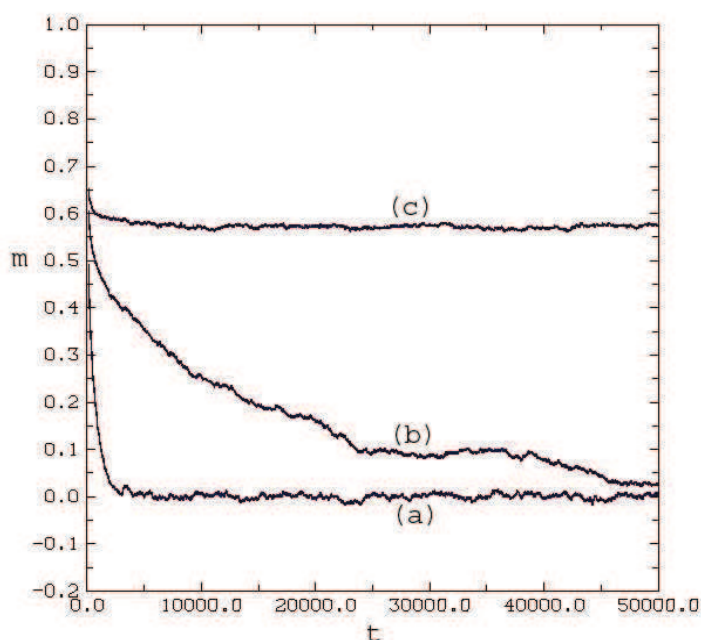Fig. 2. The magnetization versus time in the two-layer Ising model. for 3 states. a: K=0.304 ($K<K_c$), τ=3500. b: K=0.310 ($K=K_C$), τ=46000. c: K=0.313 ($K>K_c$), τ=4000. (each layer has 2500×2500 sites, start from homogeneous initial state "all +1", time steps = 50000)

One can see from these graphs that the relaxation time increases before critical point and reaches to a maximum at K_C, but after the critical point, τ decreases rapidly. So, in the

critical point, the system last a long time to stabilized. Hence, the critical point may be obtained from the graph of τ vs. K (Fig. 3). The obtained critical point from this graph is 0.310 for the two-layer Ising model.
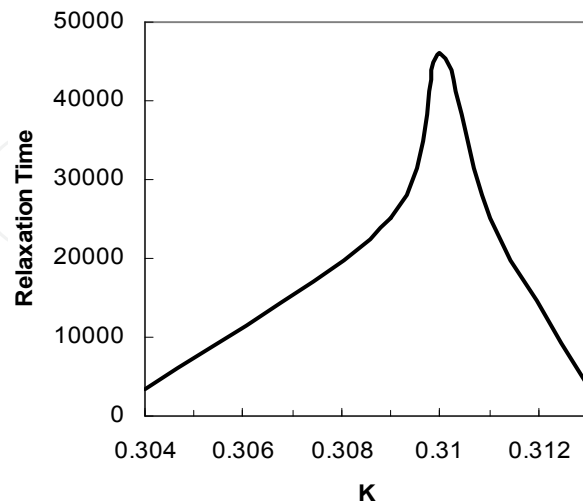

Fig. 3. The relaxation time obtained from Figure 1 versus K for the two-layer Ising model. The maximum appears at K=Kc

In our approach, we have calculated the thermodynamic quantities after thermalization of the lattice. In other words, first we let the system reaches to a stable state after some time step ($t=\tau$), and then to be updated up to the end of the automata (t=50000). For example to calculate the average value of magnetization per spin ($<m>$), one should add all values of m from the relaxation time up to the end of the automata (or end of the time step) and divide the result to number of steps. The other way for calculation of the critical point is the usage of $<m>$. By drawing the graph of $<m>$ vs. K, we may also obtain K_C. Fig. 4 shows the results
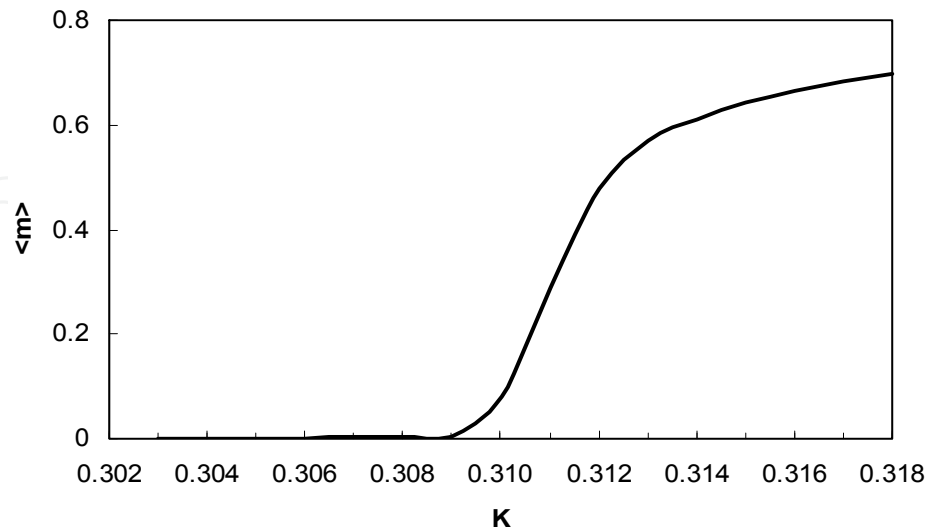

Fig. 4. $<m>$ versus coupling coefficient (K) for the two-layer Ising model. The average value for each K is calculated after its relaxation time. (data are the results for the lattice that each layer has 2500×2500 sites, starting from the homogeneous initial state with all +1, time steps = 50000)

of such calculation. As it is seen, before critical point ($K<K_C$), $<m>=0$ and after that ($K> K_C$), $<m>\neq 0$. The obtained values of the critical point from this approach is K_C =0.310 for the two-layer Ising model.

For calculation of χ for each K, first we have calculated the value of $(m-<m>)^2$ in each time step. Then these values are averaged in a same way explained above. According to eq. 8 this average could be used for computation of χ. Using eq. 9 for calculation of the specific heat (C), we have done it in a same way described above. Figures 5 and 6 show the graphs of χ vs. K and C vs. K, respectively, for the two-layer Ising model. These graphs are the other ways for obtaining the critical point. The maximum of these graphs indicates the critical point. The obtained value for K_C from these graphs is 0.310 for the two-layer Ising model.
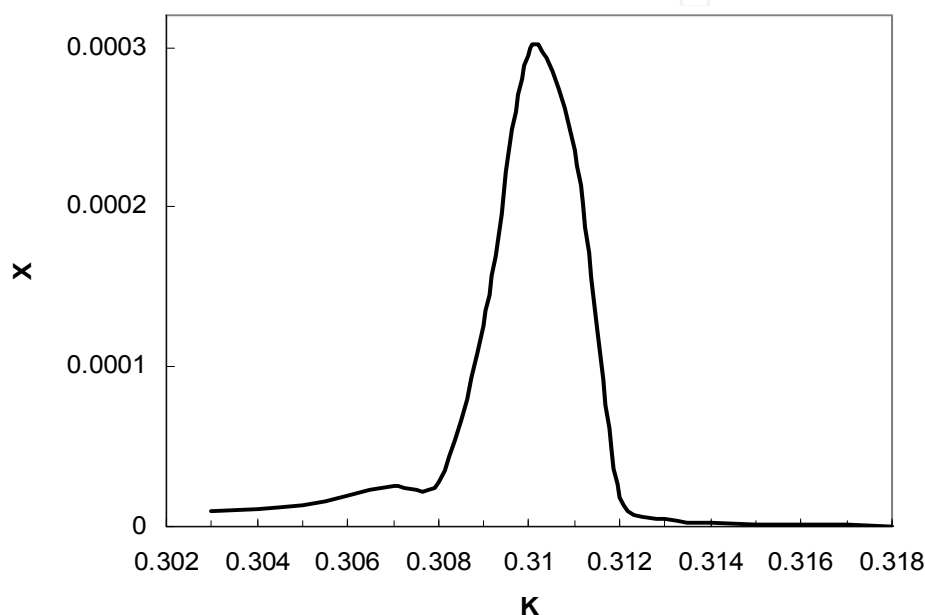

Fig. 5. Magnetization susceptibility per spin (χ) versus K for the two-layer Ising model. (The calculated data are the results for the lattice for which each layer has 2500×2500 sites, starting from the homogeneous initial state with all spins up, time steps = 50000)

3. Isotropic two-layer 3-state Potts model

Although we do not know the exact solution of the Potts model for any two-layer at present time, a large amount of numerical information has been accumulated for the critical properties of the various Potts models. Consider a two-layer square lattice with the periodic boundary condition, each layer with p columns and r rows. Each layer has then $r \times p$ sites and the number of the sites in the lattice is $2 \times r \times p = N$. We consider the next nearest neighbor interactions as well, so the number of neighbors for each site is 5. For any site we define a spin variable $\sigma^{1(2)}(i,j) = 0, \pm 1$ so that $i = 1,...r$ and $j = 1,...,p$. The configurational energy of a standard 3-state Potts model is given (Asgari et al., 2004) as:

$$\frac{E(\sigma)}{kT} = \sum_{i=1}^{r,*}\sum_{j=1}^{p,*}\sum_{n=1}^{2} -\{K_x\delta_{\sigma^n(i,j),\sigma^n(i+1,j)} + K_y\delta_{\sigma^n(i,j),\sigma^n(i,j+1)} + K_z\delta_{\sigma^1(i,j),\sigma^2(i,j)}\} \tag{14}$$
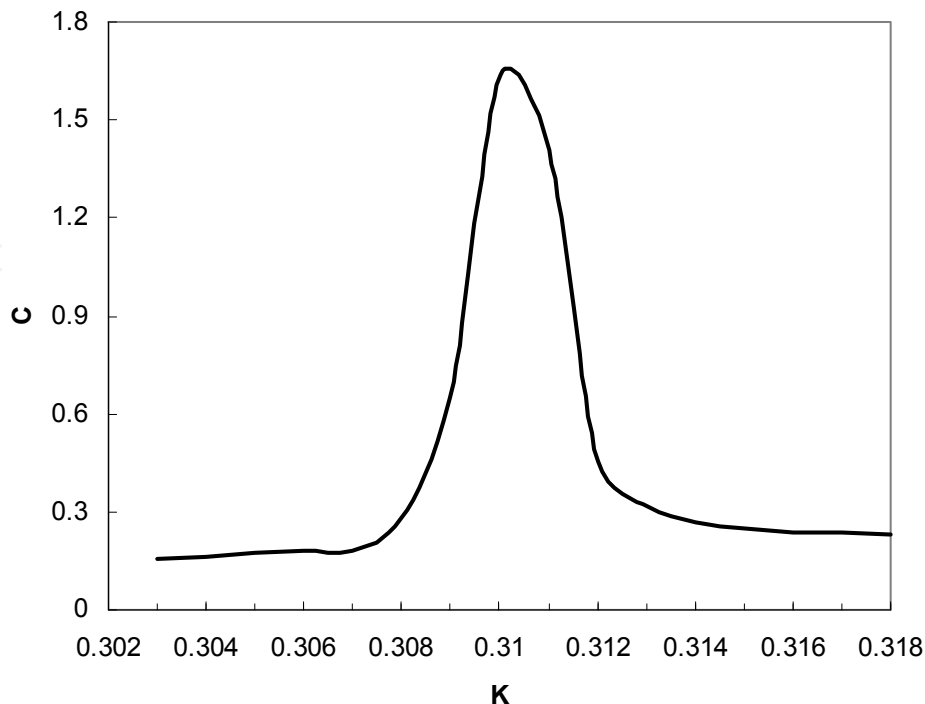
Fig. 6. Specific Heat per spin (*C*) versus *K* for the two-layer Ising model. (The calculated data are the results for the lattice for which each layer has 2500×2500 sites, starting from the homogeneous initial state with all spins up, time steps = 50000)

Where

$$\delta_{i,j} = 1 \text{ for } i = j$$
$$\delta_{i,j} = 0 \text{ for } i \neq j$$

(15)

and * indicates the periodic boundary condition and K_x and K_y are the nearest-neighbor interactions within each layer in *x* and *y* directions, respectively, and K_z is the interlayer coupling. Therefore, the configurational energy per spin is

$$e = \frac{E(\sigma)}{kTN}$$

(16)

and the general equations (5-9) are applicable to this model. For quantitative computation of the critical temperature of a two-layer 3-state Potts model, we considered the isotropic ferromagnetic case which $K_x = K_y = K_z \geq 0$. We have used a two-layer square lattice that each layer has 1500×1500 sites and to reduce the finite size effects the periodic boundary condition is used. Each site can have a value of +1, -1 or zero. We used the Glauber method with checkerboard approach to update the sites. Namely, each layer is like a checkered surfaces and at first, the updating is done for the white parts of the first layer. Then the black ones are updated. After which, this approach is done for the second layer. The updating of +1 spins is based on the probabilistic rules. The probability that spin of one site will be +1 (p_i^+) is given by

$$p_i^+ = \frac{e^{-\beta E_i^+}}{e^{-\beta E_i^+} + e^{-\beta E_i^-} + e^{-\beta E_i^0}} \tag{17}$$

Hence, probability that a given spin to be -1 (p_i^-) is

$$p_i^- = \frac{e^{-\beta E_i^-}}{e^{-\beta E_i^+} + e^{-\beta E_i^-} + e^{-\beta E_i^0}} \tag{18}$$

and for the zero state we have,

$$p_i^0 = 1 - (p_i^+ + p_i^-) \tag{19}$$

where

$$
\begin{aligned}
E_i^{\pm,0} = &-K_x \left\{ \delta_{\sigma^n(i,j),\sigma^n(i+1,j)} + \delta_{\sigma^n(i,j),\sigma^n(i-1,j)} \right\} \\
&-K_y \left\{ \delta_{\sigma^n(i,j),\sigma^n(i,j+1)} + \delta_{\sigma^n(i,j),\sigma^n(i,j-1)} \right\} \\
&-K_z \left\{ \delta_{\sigma^n(i,j),\sigma^{n'}(i,j)} \right\}
\end{aligned} \tag{20}
$$

and

$$
\begin{aligned}
\sigma^n(i,j) &= +1 \text{ for } E_i^+ \\
\sigma^n(i,j) &= -1 \text{ for } E_i^- \\
\sigma^n(i,j) &= 0 \text{ for } E_i^0
\end{aligned} \tag{21}
$$

It should be mentioned that in our approach, first we construct the probability matrix according to Eqs. (17-20) for different states of a cell in such a way that for each state it is sufficient to refer to the probability matrix and use the proper value of the probability. This leads to prevent similar calculations.

When we start the CA with the homogeneous initial state (namely, all sites have spin up or +1), before the critical point (K_C), the magnetization per spin (m) will decay rapidly to zero and fluctuate around that point. After the critical point, m will approach to the nonzero point and fluctuate around it and with increasing of K, the magnetization per spin will go toward its initial state (i.e. $m = +1$). But at the critical point, m will decay very slowly to zero with a great fluctuation. For each value of K, the time that m reaches to a special value and starts to fluctuate, is called the relaxation time (τ). On the other hand, the relaxation time is the time that system is thermalized. The value of τ can be obtained from the graph of m versus t. So one can see from this graph that the relaxation time increases before the critical point and reach its maximum at K_C, but after the critical point, τ decreases. So, in the critical point, the system last for long time to stabilize. Hence, the critical point could be obtained from the graph of τ versus K (Fig. 7).

Another way to get the critical point is the usage of the thermodynamic quantities after thermalization of the lattice. In another word, first we let the system to reach to a stable state after some time step ($t = \tau$). Next we let the system to be updated to the end of the automata
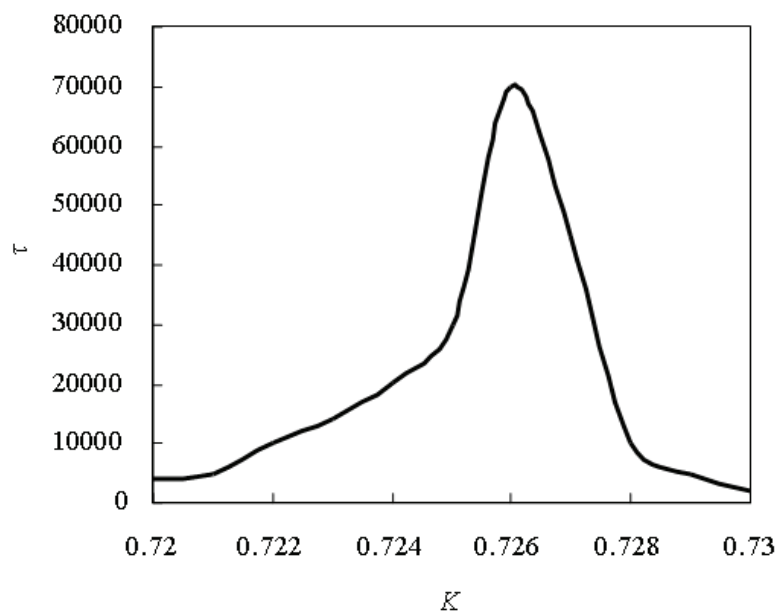
Fig. 7. Relaxation time (τ) versus coupling coefficients (K). (calculated data are the results of the lattice with 1500×1500 sites in each layer, start from homogeneous initial state with all of the spins up, time steps = 100000)

($t = 100000$). For example, to calculate the average value of magnetization per spin ($<m>$), one should add all of values for m from the relaxation time to the end of the automata (or end of the time step) and divide the result to the numbers of steps. By drawing the graph of $<m>$ versus K, we could get K_C. In this graph, for $K < K_C$, the value of $<m>$ lies around zero. But it becomes nonzero at $K=K_C$, after which, its value increases gradually. For calculation of the susceptibility per spin χ (eq. 8), for each K, first we calculated the value of $(m- <m>)^2$ in each time step. Then these values are averaged by the same method explained above. Also the calculation of the specific heat C (eq. 9), may be done by a similar way. The graphs of χ versus K and C versus K, are another approach to obtain the critical point. The maximum of such graphs gives the critical point.

The result of such calculations are shown in figures 8-10 for the simplest case of the two-layer 3-state Potts model when $K_x=K_y=K_z=K \geq 0$. The obtained value for the critical point is 0.726 for this case.

4. Constructing the critical curve for anisotropic two-layer models

The previous approach could easily be used for calculation critical point of anisotropic two-layer Ising and Potts models which have different interlayer coupling coefficients ($K_x \neq K_y \neq K_z$) (Asgari & Ghaemi, 2006 and Asgari & Ghaemi, 2008). The critical points that are obtained for the two-layer Ising model in the case of different values of $\xi = K_z/K_x$ and $\sigma = K_y/K_x$ are given in Table 1.

The results are compared with other numerical methods and it is shown that they are in good agreement. So, this comparison confirms the reliability of our approach. In the next step, we have fitted the obtained results which are in Table 1 in order to get a general ansatz equation for the critical point for the anisotropic two-layer Ising model in terms. The results are compared with other numerical methods and it is shown that they are in good
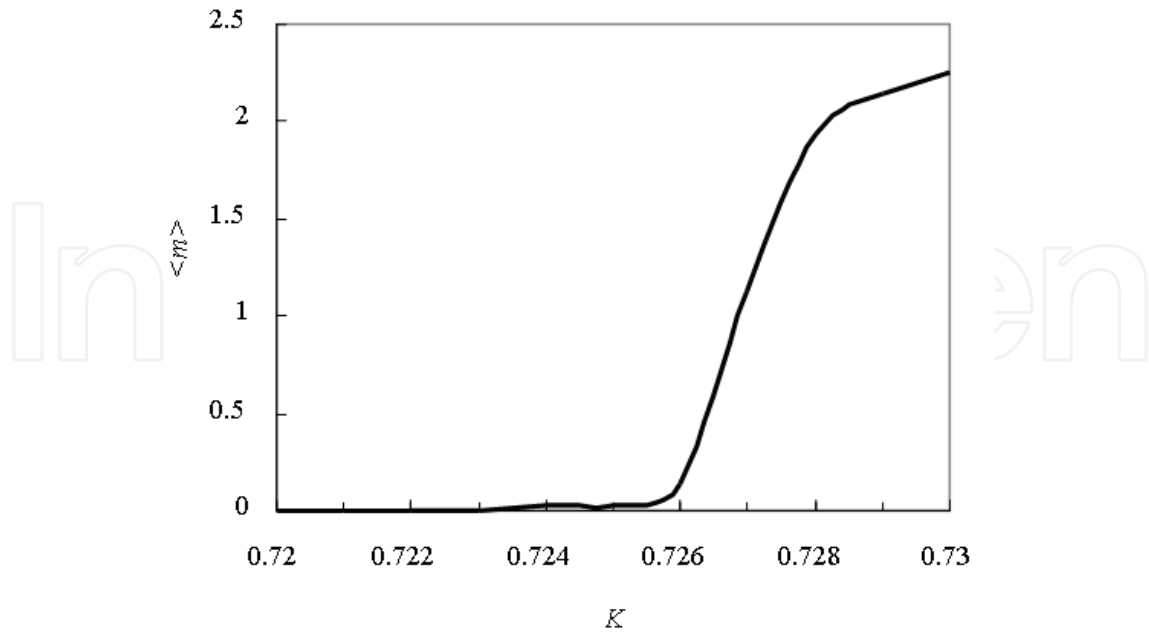
Fig. 8. <*m*> versus coupling coefficients (*K*). (calculated data are the results of the lattice with 1500 × 1500 sites in each layer, start from homogeneous initial state with all of the spins up, time steps = 100000)
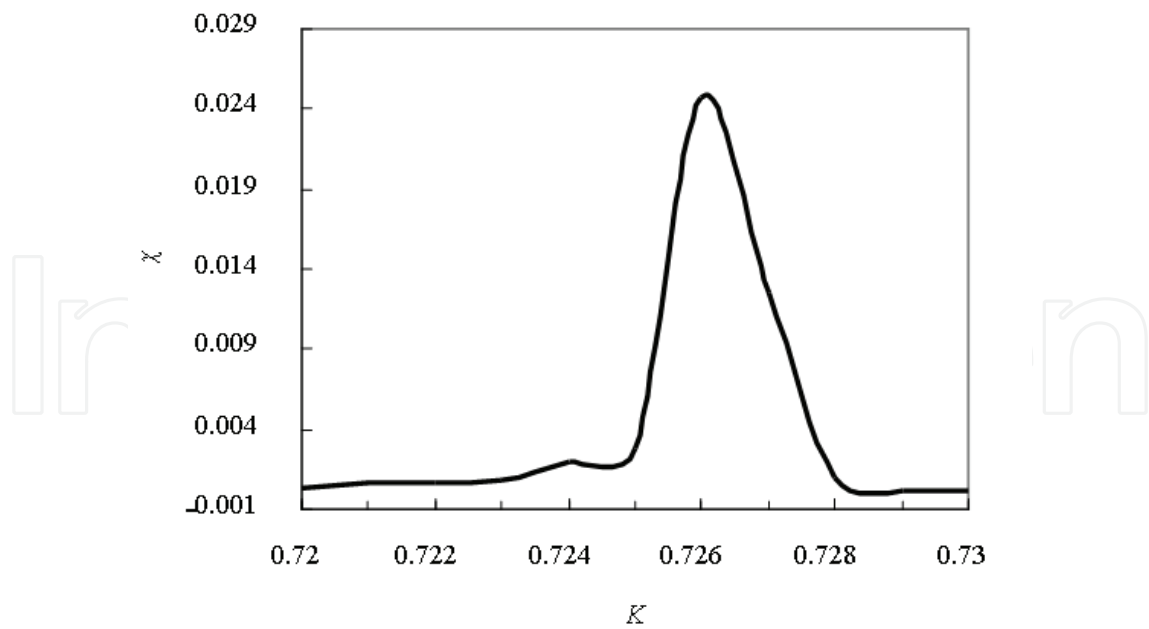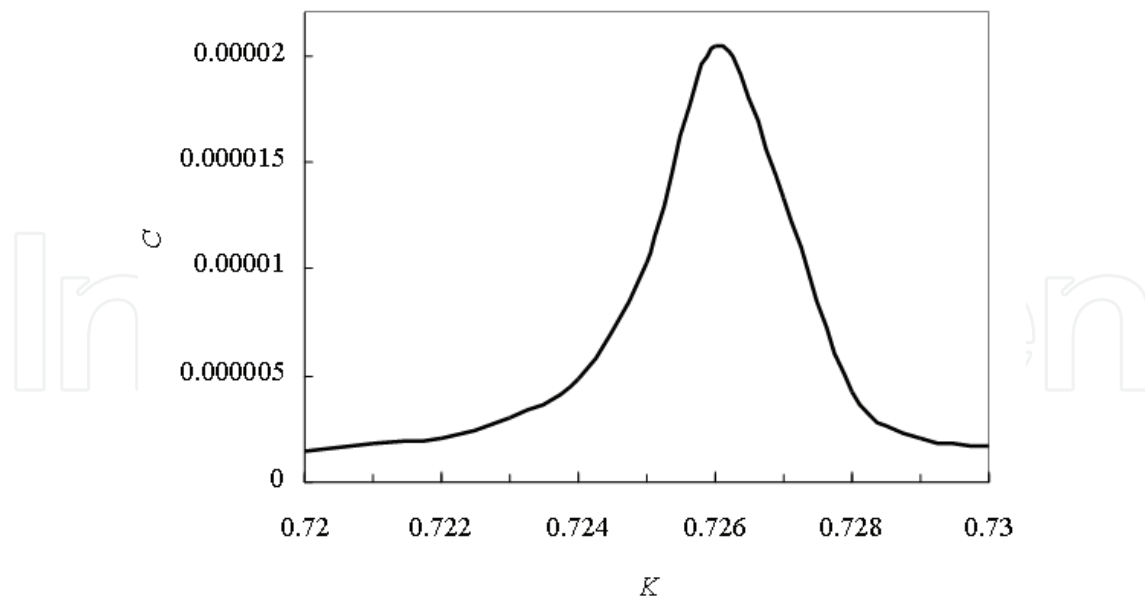

Fig. 9. Magnetization susceptibility per spin (*χ*) versus *K*. (calculated data are the results of the lattice with 1500 × 1500 sites in each layer, start from homogeneous initial state with all of the spins up, time steps = 100000)

Fig. 10. Specific Heat per spin (*C*) versus *K*. (calculated data are the results of the lattice with 1500×1500 sites in each layer, start from homogeneous initial state with all of the spins up, time steps = 100000)

agreement. So, this comparison confirms the reliability of our approach. Furthermore, it is clear from the graph of M versus t (Fig. 1) that the critical point could be easily obtained with high precision using the CA approach. In the next step, we have fitted the obtained results which are in Table 1 in order to get a general ansatz equation for the critical point for the anisotropic two-layer Ising model in terms of inter- and intra-layer interactions (ξ and σ) as,

$$K_C^{-1} = a + b\xi^{1/2} + c\sigma^{1/2} \tag{22}$$

where, a = 0.170937($\pm$0.002708), b = 0.724762($\pm$0.003046), and c = 2.19985($\pm$0.004167). This equation could be a reliable way to investigate the critical point for the anisotropic ferromagnetic two-layer Ising model by considering the nearest-neighbor interactions within each layer in the x and y directions and also the inter-layer coupling. So, having the desired values of ξ and σ, one could obtain the critical point for this model with acceptable precision. In the next step, we have done similar calculation to obtain the critical points for the anisotropic two-layer Potts model which is shown in Table 2.

Some of the results are compared with the recent transfer matrix method and it is shown that they are in good agreement. This comparison shows the reliability of our approach. The results are obtained from the graph of M versus t with high precision (see for example Fig. 2). Then, the obtained results have been fitted in order to obtain a general ansatz equation for the critical point for the anisotropic two-layer Potts model in terms of inter- and intra-layer couplings (ξ and σ) as follow,

$$K_C^{-1} = a + b\xi^{1/2} + c\sigma^{1/2} \tag{23}$$

where a = 0.162203($\pm$0.001257), b = 0.246394($\pm$0.003882), and c = 0.800764($\pm$0.003190). This equation seems to be a useful expression in order to calculate the critical point for the

anisotropic two-layer Potts model in the lack of a general equation in terms of the nearest-neighbor interactions within each layer in the x and y directions and also the interlayer coupling.

K_z / K_x ╲ K_y / K_x	0.1	0.4	0.7	1.0	1.3
0.1	0.896	0.583	0.465	0.395	0.349
	0.879 a	0.582 a	0.464 a	0.397 a 0.3977 b	0.348 a
0.4	0.747	0.503	0.408	0.352	0.312
	0.763 a	0.510 a	0.413 a	0.354 a 0.3541 b	0.315 a
0.7	0.678	0.463	0.380	0.328	0.291
	0.686 a	0.465 a	0.381 a	0.330 a	0.293 a
1.0	0.639	0.436	0.357	0.310	0.276
	0.651 a	0.436 a	0.359 a	0.311 a 0.3117 b	0.277 a
1.3	0.608	0.414	0.341	0.296	0.265
	0.629 a	0.417 a	0.343 a	0.298 a	0.267 a

[a] From the transfer matrix method (Ghaemi et al., 2003).
[b] From the corner transfer matrix renormalization group method (Li et al., 2001)

Table 1. The critical points for the two-layer Ising model.

K_z / K_x ╲ K_y / K_x	0.001	0.01	0.1	0.5	1.0
0.001	5.23	4.08	2.43	1.37	1.00
0.01	4.60	3.73	2.35	1.35	0.98 0.974860[a]
0.1	3.48	3.00	2.06	1.25	0.92 0.902499[a]
0.5	2.85	2.34	1.64	1.05	0.80 0.795385[a]
1.0	2.47	2.14	1.44	0.94	0.72 0.726306[a]

[a] From the transfer matrix method (Mardani et al., 2005)

Table 2. The critical points for the 3-states two-layer Potts model

There are some features which can be mentioned here with the physical aspects according to eqs.22-23. It is shown that the critical point is proportional to ξ and σ in such a way that it increases when the value of ξ or σ decreases. As we have mentioned in earlier work (Asgari & Ghaemi, 2006), it is possible to increase the precision of the calculation by increasing the number of lattice size in order to make the system to have less fluctuation and so, determination of the critical point will be easier. Also, it should be noted that the number of

time steps should be high enough to determine the critical point especially in the case of fourth and more digits after the decimal point. However, it is clear that increasing the number of time steps and lattice size lead to decreasing the program rate. One way is to tabulate the probabilities in eqs. (17-20) and refer to such a table for each update and find the desire values for different probabilities in order to decrease the computational time. Also, parallel processing on cluster computers for the case of a large lattice size is another way to increase the program rate. The advantage of defined approach for the calculation of the critical point using the probabilistic CA is the possibility to get digits after the decimal point like fourth and more digits with higher precision.

Finally, it should be considered that it is possible to extend this approach to other lattice models such as triangular, hexagonal, and also other models like multi-states two-layer Potts model, 3-D Ising model, and asymmetric cases in order to obtain a general equation in the lack of the exact solution.

5. Calculation of the shift exponent

A shift exponent (φ) describes the deviation of the critical temperature from the critical temperature for the decoupled limit ($Kz = 0$). Some scaling theories were constructed to obtain the shift exponent (Oitmaa & Enting, 1975; Lipowski, 1998; Horiguchi & Tsushima 1997; Abe, 1970; and Suzuki, 1971). It was shown that for the two-layer model there is a relation between the critical point and the shift exponent as follow

$$T_C(\xi) - T_C(0) \propto \xi^{1/\varphi} \tag{24}$$

These theories predict that when the intra-layer interactions are the same in each layer, then $\varphi = \gamma$, where γ is the critical exponent describing divergence of susceptibility upon approaching the critical point (Abe, 1970; and Suzuki, 1971). Also it was mentioned that
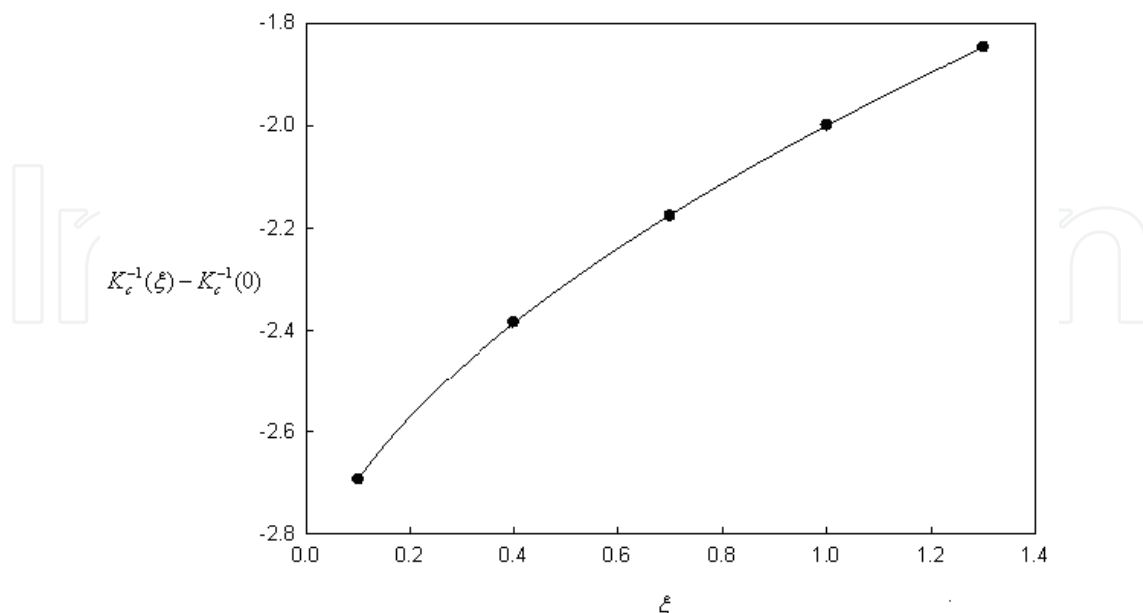

Fig. 10. The plot of $K_C^{-1}(\xi) - K_C^{-1}(0)$ versus ξ for the two-layer Ising model in the case of the equal intra-layer interactions ($K_x = K_y$)

when the intra-layer couplings changes in each lattice, then $\varphi = \gamma/2$. There has been several attempts to check these theories according to which some model gives good agreement and others show significant deviations (Lipowski, 1998 and Abe, 1970).

First, we have estimated the shift exponent for the two-layer Ising model in the case of equal intra-layer interactions. It was done considering following relation and the data of Table 1,

$$K_C^{-1}(\xi) - K_C^{-1}(0) \propto \xi^{1/\varphi} \tag{25}$$

Fig. 10. shows the plot of the left hand side of the relation (25) versus ξ. Then the results were fitted with a power equation and it was found that in this case the value of φ is 1.756($\pm$0.0078) which is in good agreement with the other works (Lipowski, 1998).

This result is also in agreement with the arguments that the two-layer Ising model is in the same universality class as the two-dimensional Ising model with $\varphi = \gamma = 1.75$. Thereafter, we extend this calculation to the case of different intra-layer interactions. The obtained results for the shift exponent are shown in Table 3 which considerably different from those predicted by others. At present we cannot say in which point these scaling arguments are wrong but clearly they require reconsideration.

σ	Φ
0.1	2.807
0.4	2.066
0.7	1.906
1.0	1.756

Table 3. The shift exponent for the two-layar Ising Model (the exact value for K_C is 0.440687).

However, the results could be fitted into a rational ansatz equation in terms of intra-layer interactions (σ) as

$$\varphi = \frac{a_0 + \sigma}{a_1 + a_2\sigma} \tag{26}$$

where $\sigma = K_y/K_x$ and the universal coefficients are $a_0 = 0.1803(\pm0.001349)$, $a_1 = 0.0399(\pm0.000451)$, and $a_2 = 0.5995(\pm0.003601)$. As shown in Fig. 11, eq. (26) has a decay form and covers all calculated data for σ ≤ 1.

In this step we have calculated the shift exponent for the two-layer Potts model. In the case of equal intra-layer interactions we have used the relation (25) and the data of Table 2 in order to calculate the shift exponent. The value for the shift exponent after fitting with a power equation is 1.582($\pm$0.0128) which differs from the obtained value for the two-layer Ising model. This result shows that the two-layer Potts model is not in the same universality class as the two-dimensional and two-layer Ising model. We have done the calculation for different values of the intra-layer couplings. The results are shown in Table 4.

These results could be fitted into a rational ansatz equation in terms of the intra-layer couplings (σ) as

$$\varphi = \frac{b_0 + \sigma}{b_1 + b_2\sigma} \tag{27}$$

where $\sigma = K_y/K_x$ and the universal coefficients are $b_0=0.0630(\pm0.000166)$, $b_1=0.0181(\pm0.000103)$, and $b_2=0.6547(\pm0.002691)$. As shown in Fig. 12, eq. (27) has also a decay form and covers all calculated data for $\sigma \leq 1$.
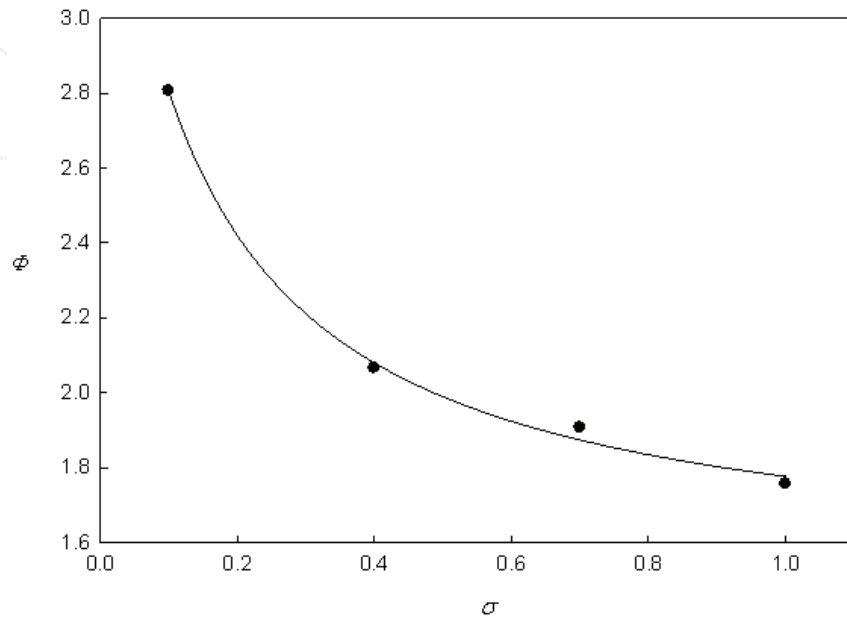

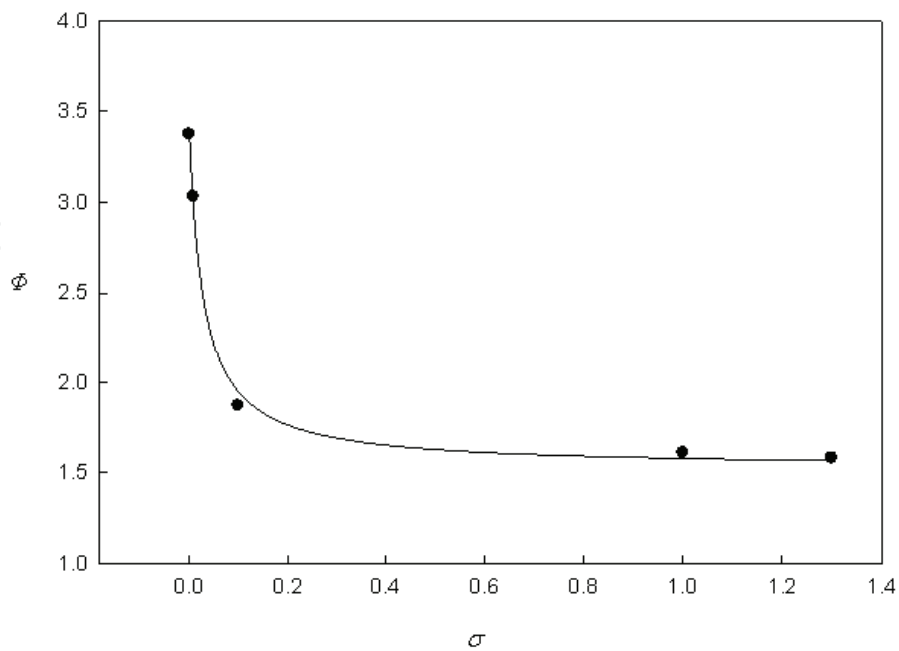Fig. 11. The Plot of φ versus σ for the two-layer Ising model

Fig. 12. The Plot of φ versus σ for the 3-states two-layer Potts model

σ	Φ
0.001	3.376
0.01	3.031
0.1	1.871
0.5	1.612
1.0	1.582

Table 4. The shift exponent for the 3-states two-layer Potts model the exact value for K_C is 1.005052).

6. Reference

Abe, R. (1970). *Prog. Theor. Phys.* 44 339.

Aktekin, N. (1999). *Annal Review of computational Physics* VII. Edited by Staufer, D., World Scientific Publishing Company 1-23

Allan, G.A.T. (1970). *Phys. Rev. B.* 1, 352

Angelini, L., Carappo, D., Pellicoro, M., Villani, M. (1995). *Physica A.* 19, 447

Angelini, L., Carappo, D., Pellicoro, M., Villani, M. (1997). *Physica A.* 237, 320

Asgari, Y., Ghaemi, M., Mahjani, M.G. (2004) *Lecture Notes in Computer Science.*, 3305, 709-718

Asgari, Y.; Ghaemi M.; (2006). *J. Theo. Comp. Chem.*, 2, 141-150

Asgari, Y.; Ghaemi M.; (2008). *Physica A,* , 387, 1937–1946

Ballentine, L.E. (1964). *Physica*, 30, 1231

Binder, K. (1974). *Thin Solid Films.* 20, 367

Creutz, M. (1986). *Annals of physics.* 167, 62-76

Domany, E., Kinzel, W. (1984). *Phys. Rev. Let.* 53, 4, 311-314

Ghaemi, M., Ghannadi, M., Mirza, B. (2003). *J. Phys. Chem. B.* 107, 829-831

Ghaemi, M., Mirza, B., Parsafar, G.A., (2004). *J. Theor. & Comp. Chem.* 3, 217-224.

Glauber, R.J.: J. Math. Phys. (1963) 4, 294

Glotzer, S.C., Stauffer, D., Sastry, S. (1990). *Physica A* 164 1-11.

Herrmann, H. J. (1986). *J. Stat. Phys.* 45, 145

Hilfer, R., Biswal, B., Mattutis, H.G., Janke, W. (2003). *Phys. Rev. E* 68 046123.

Horiguchi, T., Lipowski, A., Tsushima, N. (1996). *Physica A.* 224, 626

Horiguchi, T. and Tsushima, N. (1997). *Physica A* 238

Huang, K. (1987). *Statistical mechanics.* John Wiley and Sons, 2nd Edition,

Janke, W. (1998). *Physica A* 254 164-178.

Jan, N.(1990). *J. Physique.* 51, 201

Kinzel, W. (1985). *Z. Phys. B.* 58, 229-244

Kremer, S. and Wolf, D.E. (1992). *Physica A* 182 542-556.

Li, Z.B., Shuai, Z., Wang, Q., Luo, H.J., Schulke, L. (2001). *J. Phys. A.* 34, 6069-6079

Lipowski, A. (1998). *Physica A* 250 373-383.

Lipowski, A., Suzuki, M. (1998). *Physica A.* 250, 373

MacIsaac, A.B. (1990) *J. Phys. A* 23 899-903.

Mardani, T. , Mirza, B., Ghaemi, M. (2005). *Phys. Rev. E* 72 026127.

Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H., Teller, E. (1953). *J. Chem. Phys.* 21, 1087

Moukarzel, C. and Parga, N. (1989). *J. Phys. A* 22 943.

Newman, M.E., Barkema, G.T. (2001). *Monte Carlo Methods in Statistical Physics*. Oxford University Press Inc., New York, Reprinted. Chap. 3-4.

Oitmaa, J., Enting, G. (1975). *J. Phys. A.* 8, 1097

Onsager, L. (1944). *Phys. Rev.* 65, 117

Pomeau, Y. (1984). *J. Phys. A.* 17, 415

Stauffer, D. (2000) . *Comp. Phys. Comm.* 127 113-119.

Stauffer, D. (1997) . *Int. J. Mod. Phys. C* 8 6, 1263-1266.

Suzuki, M. (1971). *Prog. Theor. Phys.* 46 1054.

Toffoli, T., Margolus, N. (1990). *Physica D.* 45, 229-253

Vichniac, G. (1984). *Physica D*10. 96-115

Wosiek, J. (1994). *Phys. Rev. B.* 49, 15023

Wu, F.Y. (1982). *Rev. Mod. Phys.* 54, 235

Zabolitzky, J. G. and Herrmann, H. J. (1988). *J. Comp. Phys.* 76 426-447.

Zheng, B. (1998). *Int. J. Mod. Phys. B* 12 14, 1419-1484.
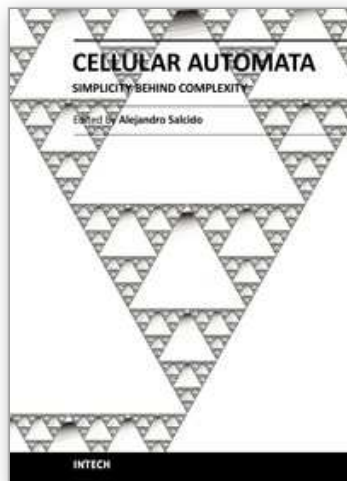
Cellular Automata - Simplicity Behind Complexity

Edited by Dr. Alejandro Salcido

Cellular automata make up a class of completely discrete dynamical systems, which have became a core subject in the sciences of complexity due to their conceptual simplicity, easiness of implementation for computer simulation, and their ability to exhibit a wide variety of amazingly complex behavior. The feature of simplicity behind complexity of cellular automata has attracted the researchers' attention from a wide range of divergent fields of study of science, which extend from the exact disciplines of mathematical physics up to the social ones, and beyond. Numerous complex systems containing many discrete elements with local interactions have been and are being conveniently modelled as cellular automata. In this book, the versatility of cellular automata as models for a wide diversity of complex systems is underlined through the study of a number of outstanding problems using these innovative techniques for modelling and simulation.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

INTECH
open science | open minds