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Cellular Automata-based Optimization of the Spin-Glass Discrete Problem in a Ferromagnetic and Anti- ferromagnetic Material

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Abstract: According to the discussion about the discrete characters of Spin glass on Ising model, the feasibility to study spin glass based on cellular automata is demonstrated, while a method searching for lower energy state of the spin glass based on Cellular Automata is proposed. This method achieves energy optimization of the material and calculate the total energy of the system by programming the cellular automata with Visual C + + and using the Ising model and the Neumann's defining for neighbor node. Among the experiment of cold compress spin, the natural optimization process of energy can be simulated. When the temperature is higher than Curie point, the internal magnetic field of ferromagnetic materials is in a state of disorder and becomes a paramagnet. This phase change is reversible in nature. While the magnetic field of anti-ferromagnetic materials tends to be empty with the temperature decreasing. The result shows that cellular automata is much more superior compared with simulated annealing algorithm, which may not only introduce a new way to study magnetic Spin glass, but also explore other optimization problems, such as the ground state problem of SDN, TSP, peddler problem, satisfiability problem and so on.

Keywords: Cellular Automata; Spin-Glass; Ising Model; Local Optimization; Simulated Annealing Algorithm

1 Introduction

This paper discusses a simulation algorithm--cellular automata, which will be used to research the spin glass of orientation disordered system. That may be applied in many fields.[1,2] The reason of choosing cellular automata mainly lies in that the cellular automata itself is a random discrete model with complicated structure (from an historical viewpoint). It is a kind of discrete grid dynamic model， whose time, space and state are all discrete, and the spatial interaction and causality on time are completely specified in terms of a local relation. The traits of cellular automata such as "from bottom to top" approach, strong complicated computing capability, inherent parallel computing capability, highly dynamic characteristic and spatial concept, etc., have made it very strong on spatial-temporal evolution modeling of the complex system. cellular automata has shown thoroughly the essence of complexity science that "the complicated structure comes from the interaction of the simple subsystem" [3-6]. Therefore, to do a research on spin-glass with cellular automata may conform to our original intention of recognizing complicated system.

Being based on this and inheriting the opinion of Margenstern(1999)[7] that all the NP-complete problems can be resolved by cellular automata in hyperbolic plane, as well as being assisted by the discussion on spin-glass ground state employing Ising model, this article argues that the Ising model can be simplified into NP completed problems. In other words, the discrete characteristic of spin-glass helps us to resolve this problem with cellular automata. Furthermore, it indicates that the cellular automata can simulate effectively on spin-glass ground state though a programming experiment with a group of ferromagnetic materials and anti-ferromagnetic materials. Also, on the comparison of traditional simulated annealing, it shows that cellular automata can be more effective in resolving the problem of spin-glass and suggests that cellular

automata is an ideal solution on discontinuous optimization problem.

2 RESEARCH MODEL

2.1 Ising Model

In this research on spin glass, Ising model, the statistical physics model is introduced to modeling the collective effect resulting from the interaction between two classes of particles in different states. In the magnetic-particles-formed network, there are only two possible values for the particles vector, namely +1 and −1. But the spin of the particles in +1 or −1 distribute in some part of rather than everyone of grid points in the probability of $p(0 \prec p \prec 1)$.[8] For the sake of research, the author made the following assumptions:(1)Spin particles arrange in square or cube; (2)Treat spin particles as unit vector, in the value of +1 or −1; (3)Interaction only exists in a pair of neighboring spin particles; (4)The interactive force between each pair of spin particles (i,j) is constant.

Given that each grid point is affected by both the closest and secondary closest neighbors, the total energy of the system is calculated in the following formula.

$$E = \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij} S_i S_j \qquad \textbf{(1)}$$

In formula (1), J_{ij} means the interaction between spin particles, when $J_{ij} \succ 0$, the system is in antiferromagnetism; while when $J_{ij} \prec 0$, the system is in ferromagnetism; specially, when $J_{ij}=0$, there is no interaction between the spin particles and the atoms tend to be ordered under ferromagnetism while disordered under antiferromagnetism. Here, S_i represents the magnetic moment of spin particle. If a pair of spin particles rotate in the same direction, the value of magnetic moment equals to +1 , otherwise the value of magnetic moment equals to −1 . As each pair of spin particles are twice calculated, the total energy should be divided in half. Particularly, spin particles rotate in random direction when the heater energy is more powerful than atomic interaction energy in the system.

2.2 Spin glass and max-cut problem

There is a strong association between spin glass and max-cut problem. Spin particles can be divided into two related groups in terms of magnetic moment and the system's total energy can be calculated by the following formula (2).

$$\begin{aligned} E &= \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij} S_i S_j \\ &= \frac{1}{2}\left(\sum_{i,j\in S+} J_{ij} + \sum_{i,j\in S-} J_{ij} - \sum_{\substack{i\in S+ \\ j\in S-}} J_{ij} - \sum_{\substack{i\in S+ \\ j\in S-}} J_{ij} \right) \\ &= \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij} - \sum_{\substack{i\in S+ \\ j\in S-}} J_{ij} \end{aligned} \qquad \textbf{(2)}$$

The formula (2) indicates that min E⇔ max $\sum_{\substack{i\in S+ \\ j\in S-}} J_{ij}$.

Therefore, spin glass problem can be treated as max-cut problem and Ising model is closely associated with optimization problem. Ising model is more than a physical model. It represents a class of discrete optimization problems and can be solved with discrete method such as cellular automata. Were the results of the experiment correct, cellular automata can be applied to solve the traveling salesman problem. But the traditional complicity is the local optimal achieved without any clue on the global. That is the limitation in solving the traveling salesman problem and also a greater challenge to being modeled with cellular automata. However its feasibility and significance in processing complex problems through Fadaei and Setayeshi'sapplying cellular automata in solving nuclear plant's problem.[9] Further along, this paper aimed to prove that cellular automata can solve the spin glass problem in two- dimensional space. The author emphasizes that the neighboring atoms can be defined on the base of the number of selected dimensions and the operations on cellular automata are identical in any dimension. These points on two-dimensional spin glass are different from what was discussed by Onsager[3] in 1944 through calculating the free energy in a system.

3 ISING MODEL SIMULATION BASED ON CELLULAR AUTOMATA

3.1 Experimental purpose

To demonstrate the feasibility, the author made some models to simulate the cooling process of a group of ferromagnetic and anti-ferromagnetic materials, namely simulating on the natural optimization of energy between the spin particles in cooling process. In physics, the magnetic of ferromagnetism varies with temperature and the curves in Fig 3. 1 reflect the transition[4,5].

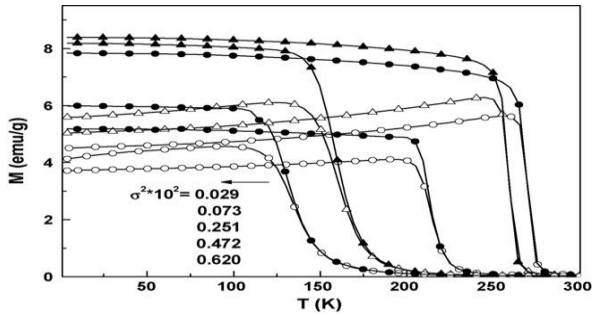

Fig 3.1 La2/3−xEuxCa1/3−ySryMnO3 Magnetic field curve varying with temperature

The curves manifest that in ferromagnetic materials, the system energy reaches minimum, the magnetic field maximum, and the system entropy S minimum when the spin particles rotate in the same direction. But the entropy S increases coupled with the temperature. At high temperature, spin particles rotate in random directions so that the higher the temperature is, the smaller the magnetic field is. Given that some texture will stabilize from chaos with descending system temperature, the author chose the fourth type of cellular automata as mentioned in the fourteenth paper listed in bibliography.

3.2 The framework

To program the cellular automata for simulation, Visual C++ is selected as the coding tool in that the class and method based programing mode is more intelligible. To achieve the energy optimization in materials, Ising model[6,10,11] and Neumann's neighboring nodes definition[12] are adopted in research. To calculate the total energy of the system, all spin particle's energy are summed up.

$$E_i = energy\_contribution\_from\_the\_i^{th}\_spin$$
$$= -J \times S_i \times (S_{above} + S_{below} + S_{left} + S_{right})$$

The framework of the system is shown in Fig3.2.

The input of the system is initial temperature and initial setup. The initial setup can be generated by a simple randomizing algorithm. The simulation system will end the program in line with the parameters CQ (convergence coefficient) and N. The process is described as the next.

Calculate and take note of the magnetic field and system total energy on each temperature node. At high temperature, each cellular is initialized to -1 or 1 (distributing uniform probability) through random function. In the experiment, a monitor is added to guarantee the simulation will be ended when the system energy reaches maximum. The monitor is ten values neighboring global energy, the gap between the maximum and minimum of the ten values will be calculated in each circle. If the gap is smaller than CQ, the counter will plus 1, else the counter will return to zero. If the counter equals N, the simulation will be ended.

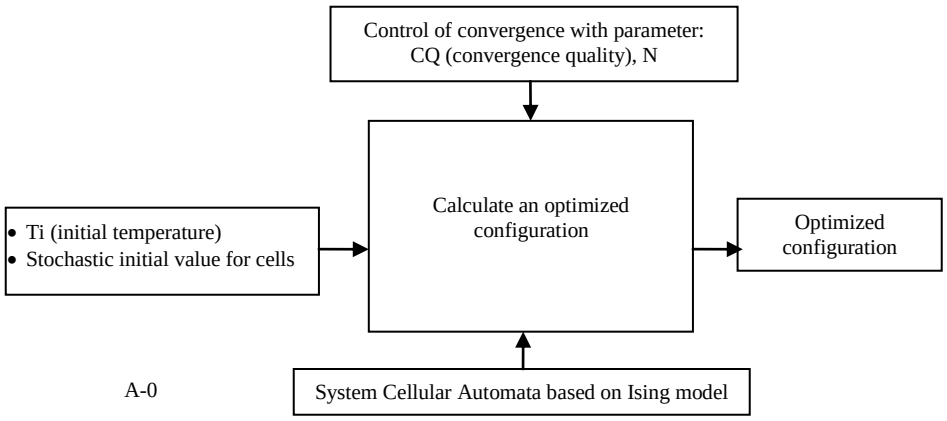

Fig3. 2 Formalisation IDEF0 of the system

4 EXPERIMENTAL RESULT

4.1 Ferromagnetism

From the magnetic field curve with variation of temperature, it is easy to tell that the magnetic field is stable at low temperature and the induction of magnetic field is in random. As shown in Fig.4.1, the experimental result demonstrate the stable magnetic field phenomenon as discussed in the 12th paper listed in the bibliography.

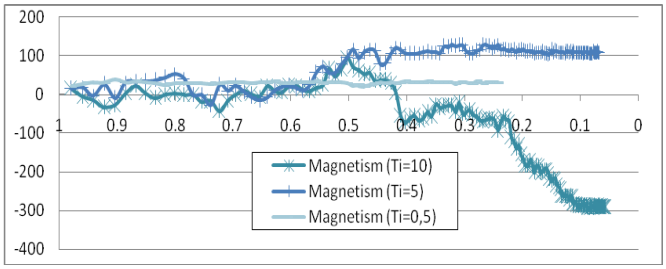

Fig.4.1 Magnetic field variation with the temperature under three different initial temperature

At high temperature, the system's magnetic field indensity is low while at low temperature, the magnetic of material tend to be stable as the system entropy is big and the system is unstable. Because the magnetizing indensity changes continuesly, it is impossible to display the curve of magnetizing rate variation.

From the decreasing curve of energy varies with temperature, it is clearly that the system stablizes quickly when the initial temperature is 0.

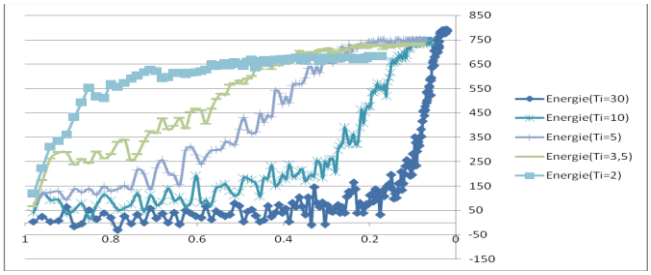

Fig4.2 System energy variation under different initial temperature

Since modeling on ferromagnetic materials, the interaction force is possitive. In Fig.4.2, it illustrates that the curve of system entropy is like a straight line if the initial temperature is 5 kelvin and for the initial temperature is 30 kelvin, the curve climbs to the top.

When the initial temperature is 10 kelvin, repeat in simulating for six times and the curves show that the energy gap between these curves amounts to about 100 joules(in Fig. 4.3 and Fig. 4.4) indicating the randomness of the experiment. Thus, these result should earn attention as the 100 joules gap is not very small against the maximum 800 joules.

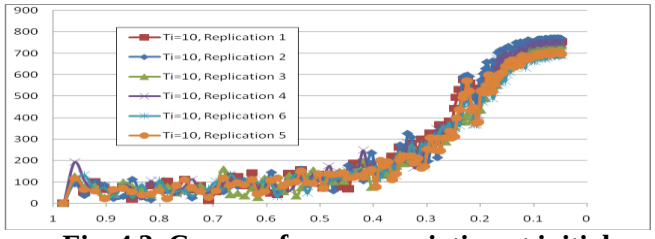

Fig. 4.3 Curves of energy variation at initial temperature 10 kelvin

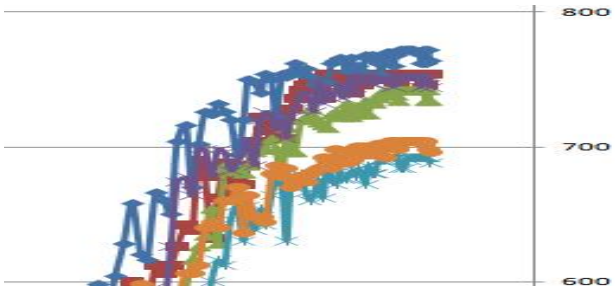

Fig. 4.4 Enlargement of the gaps between curves at initial temperature 10 kelvin

Repeat the simulation for twenty times at initial temperature 10 degree Kelven, and after caculation the formula (3) and formula (4), the curve of C_v can be drawn as the Fig. 4.5.

$$Cv = \frac{\partial \langle E \rangle}{\partial T} = \frac{\beta}{T} \cdot \frac{\partial \langle E \rangle}{\partial \beta} = \frac{\beta}{T} \cdot \frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{\beta}{T} \cdot \frac{\partial}{\partial \beta}\left(\frac{1}{Z} \cdot \frac{\partial Z}{\partial \beta}\right)$$

$$= \frac{\beta}{T} \cdot \left[\frac{1}{Z} \cdot \frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2} \cdot \left(\frac{\partial Z}{\partial \beta}\right)^2\right]$$

$$= \frac{\beta}{T} \cdot \left[\langle E^2 \rangle - \langle E \rangle^2\right]$$

$$E = \frac{1}{Z} \cdot \frac{\partial Z}{\partial \beta} = \frac{\partial Z}{Z} \cdot \frac{1}{\partial \beta} \quad (1)$$

Here: H is intensity of magnetic field, note for amperage in unit length; $Z(T)$ is called the partition function, which can be seen to be equal to $Z(T) = \sum_S e^{-\beta E_S}$; β is the inverse of temperature multiply by K_B , the Boltzmann constant,

So $\beta = \frac{1}{K_B T}$; Similarly, the magnetizing rate depends on velocity of variation of magnetic field as the following formula.

$$\begin{aligned}\chi &= \frac{\partial \langle M \rangle}{\partial H} = \beta \cdot \frac{\partial \langle M \rangle}{\partial \beta} = \beta \cdot \frac{\partial^2 \ln Z}{\partial \beta^2} \\ &= \beta \cdot \frac{\partial}{\partial \beta}\left(\frac{1}{Z} \cdot \frac{\partial Z}{\partial \beta}\right) \\ &= \beta \cdot \left[\frac{1}{Z} \cdot \frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2} \cdot \left(\frac{\partial Z}{\partial \beta}\right)^2\right] \\ &= \beta \cdot \left[\langle M^2 \rangle - \langle M \rangle^2\right]\end{aligned} \quad (4)$$

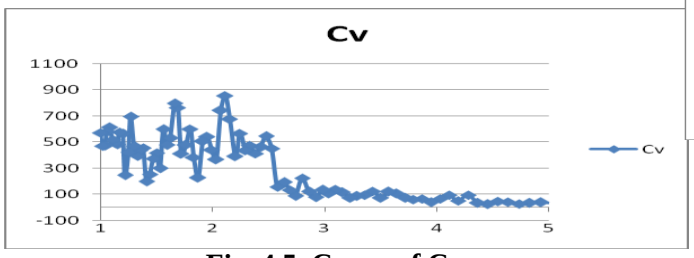

Fig. 4.5 Curve of Cv

As the Fig. 4.5 shown, there is a variation of amplitude at temperature from 1 kelvin to 2.1 kelvin due to the metastability of the system. The temperature of materials should be increased if the heat measured by means of heat capacity. As a result, the higher the heat capacity is, the higher the heat is. The emergance of the variation amplitude happens when the atoms are hindered from passing down the rotation in materials. C_v reaches the local minimum during the atoms' active movement. Then, the atoms will pass down the active movement to other atoms so as to lower the material's activeness and raise the C_v. If the atoms have no energy to pass down to other atoms, C_v arrives at the peak.

It is apparently that the curve's ceiling temperature is 2.1 kelvin, the critical temperature discovered by Curie in 1895. The Curie point or Curie temperature is named for the critical temperature at which the ferromagnetic material loses its original magnetic field. When the temperature is higher than Curie point, the inner magnetic field is disordered and the material turns into a paramagnet. As the phase transition is reversible, when the temperature is cooling down under Curie point, the original magnetic field of the ferromagnetic material is recovered. The Curie point can not be found on the magnetic variation curves because the induction of magnetic field is in random also it is impossible to draw the magnetized coefficient curves.

4.2 Anti-ferromagnetism

Anti-ferromagnetic materials are opposite to the ferromagnetic materials. It means to find out the minimum of energy rather than maximum in anti-ferromagnetic materials.

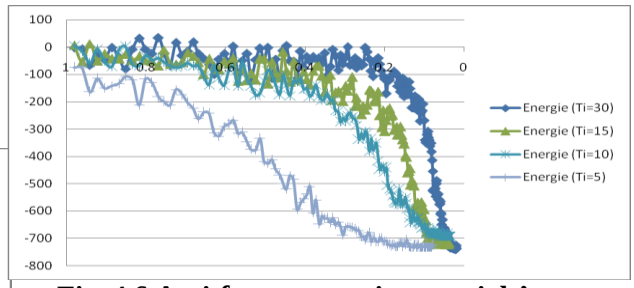

Fig. 4.6 Anti-ferromagnetic materials' energy variation curves at different initial temperature

The interaction is positive in the modeling on anti-ferromagnetic materials. The Fig. 4.6 illustrates that when the initial temperature is at about 5 kelvin, the system energy variation curve is close to a straight line and when the initial temperature is at 30 kelvin, the curve decreases to the bottom.

The Fig. 4.7 demonstrates the variation of magnetic field of anti-ferromagnetic materials at two different initial temperature. As the Fig.4.7 told, the magnetic field tends to be disordered at the beginning and when the temperature arrives at 0 kelvin, the simulation ends up with the magnetic field intensity around 0.

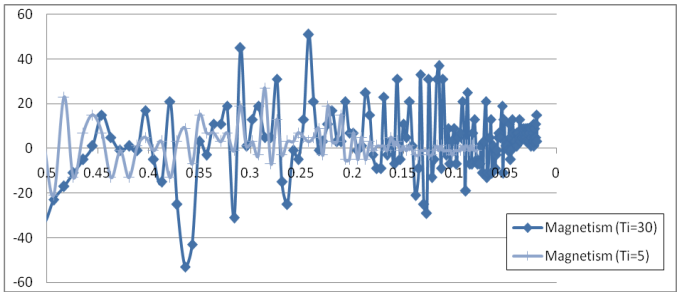

Fig. 4.7 Magnetic field variation with temperature at different initial temperature

In the experimental results, all states are the same as preset. The identical characteristics are found out in not only spin glass but also in the cellular automata simulating spin glass. By feat of the cellular automata, it is possible to solve the spin glass

problem in both ferromagnetic materials and anti-ferromagnetic materials. There findings are that in the ferromagnetic materials, the spin glass system reaches the maximum which climbs up with the increasing temperature; in the anti-ferromagnetic materials, the spin glass system arrives at the minimum which falls down with the rising temperature.

The experiment concludes that in the ferromagnetic materials modeling, the magnetic field reaches maximum with the decreasing temperature while in the anti-ferromagnetic materials modeling, the magnetic field tend to be null with the dropping temperature.

5 Cellular automata algorithm and simulated annealing algorithm

The previous experiment proves the feasibility of cellular automata in solving the spin glass discreate optimization problem. The advantage lies in the simultaneous evolution of every cellular with the decreasing temperature. the modeling is more independent as there is no need to calculate the global energy to check the necessity of every step of evolution. Comparatively, in the traditional simulated annealing algorithm, supported by " implements a Monte Carlo simulation of a 2D Ising model" (Driscoll in 2006), the system total energy should be calculated after every step of evolution so as to avoid incontrolable evolution, which makes the algorithm signifigantly limited. In the cellular automata algorithm, the only variable is the decreasing temperature. In reality, when the state of each unit is changed, it doesn't need to consider the significanse of its variation to the global. Thus, the algorithm is closer to reality. The following research focuses on the comparison of two algorithms on this modeling.

On the base of the comparison of the two algorithm, repeat modeling for 100 times at a certain temperture and compare the lenth of time of the process. For the sake of data analysis, pick up a reliable region which holding 95% values. The program keeps running untial obtain the convergence results shown as Tab.5. 1.

Tab.5. 1 Comparison of the algorithms

Experiment	Simulated anneling algorithm (100 values) (ms)	Cellular automata algorith (100 values) (ms)
Standard devition	19365,223	9649,977
Arrays	72736,6	58702,83
Limit inferior	68941,086	56811,469
Limit superior	**76532,114**	**60594,191**

Source：data from 200 simulations
Pentium(1.8GHz) confidence interval 95%

After the PC testing, the conclusion comes out that the cellular automata algorithm is quicker than simulated annealing algorithm and the cellular automata is an more effective method to solve the spin glass problem.

6 CONCLUSION

This article proves the intensive relationship between spin-glass and big cut problem. Then it undertakes a programming experimental on cellular automata by Visual C++ and gets a curve indicating magnetic field and energy changes as temperature changes in a series of ferromagnetic and anti-ferromagnetic material experiments. It proves that it's possible to resolve the problem of spin-glass with cellular automata. Also on the comparison with simulated annealing, it also gets a proof on the superiority of cellular automata in spin-glass problems. This kind of optimization with cellular automata and partial regulation demonstrated that the optimization problem can be overcome with the help of cellular automata. In the future, we will go on to probe into other optimization problem with cellular automata, such as establishing the models of TSP, pedlar problem and satisfiability problem(SAT） and so on.

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