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Critical Phenomena: Towards Modeling with Cellular Automata

Andrzej Wiśniewski
Institute of Computer Science, University of Podlasie
ul. 3 Maja, 08-110 Siedlce, Poland

Abstract. The paper presents basic description methods of critical phenomena, i.e. first-order, continuous phase transitions, and an overview of the self-organized criticality concept. In this approach an attempt is made to identify the determinant factors of modeling critical events using cellular automata.

Keywords: phase transitions, cellular automata, self-organized criticality

1 Introduction

The widespread occurrence of phase transitions in the surrounding reality is of crucial importance for all life over the world. In general, the various liquid-gas, solid-gas etc. transitions exhibit discontinuity in their physical properties while transforming from one state to another. States of the matter, magnetic features, structure etc. change as an effect of phase transitions. In any system containing liquid and gaseous phases there exists a special condition on which distinction between those phases is almost impossible. That special combination of pressure and temperature is called a critical region or critical point. In another class of systems, which evolve in such a way so as to approach a critical point and remain therein, we assume that a system exhibits a feature of self-organized criticality (SOC). That feature defines any system that takes an organized form in the absence of any external pressures. The critical events considered above may be observed in the physical or non-physical systems but using the term of phase transition to the last one is more controversial. Both considered types of the critical phenomena contain a critical point, where a small change can either push a system into a chaotic behavior or lock the system in a fixed behavior. That point is called as the Edge of Chaos.

Cellular automata, especially multi-dimensional, allow modeling many real-world phenomena, as well as abstract problems. The aim of this paper is an attempt to identify possible restrictions in the use of cellular automata for modeling critical phenomena.

2 Phase transition

The following consideration of phase change refers to the thermodynamic equilibrium. A system is physically and chemically homogenous if it is located in one state of matter. Furthermore, the systems in equilibrium state may be characterized by the functions widely known as thermodynamic potentials. All of the properties of thermodynamic systems in equilibrium state are defined by a set of factors which may be chosen from the following parameters: entropy S, temperature T, pressure p, volume V, number of molecules N and chemical potential μ. In case of a system with non-existent influence of pressure and volume we choose another parameters, i.e. for magnetic matters we take magnetic field h and magnetic moment M.

A phase change or phase transition is the transformation from one phase to another. The most differentiating characteristic of a phase transition is an abrupt change in one or more properties. That change, in particular the heat capacity, is a function of small change in an intensive parameter (thermodynamic variable), such as the temperature. The various solid-liquid-gas phase changes occur in different ways. The first Ehrenfest classification grouped phase transitions based on the continuity of chemical potential. For example, the first-order phase transition exhibits discontinuity in the first derivative of the free energy $f(T,p)$ (Helmholtz's free energy) or free enthalpy $g(T,M)$ (Gibbs' free energy), called as the thermodynamic potentials. The higher order of phase transition will be define under this scheme. As the Ehrenfest classification of phase transitions is flawed, the modern one is based on the existence or non-existence of an association of latent heat of transition. That modern approach to classification divides phase transitions into two broad categories: first- and second-order phase transitions. The first-order phase changes are those that include a latent heat. The system under that kind of transition either absorbs or sets free a fixed amount of energy. A layer between two phases, i.e. boiling water under atmospheric pressure, forms a turbulent mixture of water and vapor. The second-order phase transition or continuous phase transition has a continuous free energy function (thermodynamic potential) and a continuous first-order derivative, what affects non-existent latent heat. That kind of phase transition has some interesting features because there is a huge and long-term fluctuation of the order parameter.

As we observe a system in the critical state, we find that some characteristic system factors approach infinity. In that case a convenient description is a function in a non-analytic form e.g.: heat capacity $C \propto \tau^{\alpha}$ where $\tau = (T-T_c)/T_c$, T_c being the temperature in a critical point. The α variable is called a critical index (or critical exponent) and defines the way, in which the function $f(x)$ approaches infinity or zero. It is astonishing that critical indexes in different systems possess the same set of values with accepted level of the measurement error (sometimes rather high). After Warks, Larkin, Griffith and Kadanoff, we call that phenomenon as universality. A general idea of the universality is a thesis of grouping continuous phase transitions in a few classes (classes of universality), depending on dimensions of the system and symmetry of the ordered state. For each of the universality classes the physical variables near the critical point depend on the distance from that point. As a result, in

a class of universality all critical indexes are influenced by the variables mentioned above and dimension of the order parameter.

The next step in the development of the phase transition theory was Landau's idea that all systems (he had examined some magnetic matters) have variables whose small change results in a change of symmetry (thus to a change of the matter properties). It turned out that the critical indexes are not mutually independent. The scaling hypothesis (Rushbrook, Griffith and Widom) based on that assumption was applied by Wilson to the evaluation method of critical index values. The concept of Wilson and co-authors, named as the renormalization group method (RG), leads to the procedure of finding a critical point. Together with the scaling hypothesis it generates an association, called a scaling relation, which is satisfied by the critical indexes.

The first-order phase transition, as we considered above, contains latent heat. On the boundary between two phases there exists an interfacial layer, including defective matter (within a nucleation phase transition model) and fluctuations with a critical dimension higher than the potential barrier. That kind of systems is difficult to analyze because their dynamics is not easy to control. We assume that the universality hypothesis for first-order phase transitions is analogous (however, possibly falling within a narrow scope) to the continuous one, and ultimately will be created.

3 Self-Organized Criticality (SOC)

Self-Organized Criticality defines the critical state of a system without the need of tuning a control parameter. It means that the critical state of a system is an attractor of its dynamics. A move from a large region of the state space to a persistent smaller one (attractor) is independent from the initial conditions. That new, far from equilibrium, critical state is stable even in case of critical fluctuations. Back and co-authors [3] derive the SOC concept from the creation of avalanches on a pile of sand. In these models adding grains makes local slopes unstable and initiate avalanches, but their dimensions and moments of slide down are non-predictable. Studies of the SOC states as a phase transition, take conclusions from some observable events e.g. earthquakes or BTW models, i.e. such distributions of results that the larger event, the less frequent. The distribution of the dimension s of an avalanche may have the following mathematical form: $p(s) \propto s^{-\tau}$. If we plot the logarithm of the number of times the avalanches are found versus the logarithm of the dimension of an avalanche, we get a straight line. In general the above function is called a power law. Any system subject to the power law exposes the same structure over all scales. Both self-similarity and scale independent features are characteristic of the self-organized systems.

The published SOC models could be divided, after Frigg [11], into two basic groups. The models with stochastic dynamics working in a deterministic environment are classified into the first group of so-called "stochastic models". An example of such a system is the BTW model, forest fire, earthquake etc. The second group, so-called "quenched", consists of models with deterministic dynamics performing in random environments. Here we can mention e.g. the Bak-Sneppen

evolution model [31], or production and inventory dynamics [10]. The SOC idea has been used to model phenomena (besides given above) as diverse and impressive range as the dynamics of river network, volcanic activities, traffic jams, superconductivity, variation of stock market etc. It is interesting, but non-representative opinion, after Blanchard [11], that the SOC becomes a new paradigm of explanation of physical, social and many other phenomena. According to that paradigm, other authors [11] claim that "the world is simpler that we think" and the SOC features are ubiquitous.

It is questionable, whether the general conditions under which a physical system exhibits the SOC feature, are still unknown and from that point of view the SOC would be treated rather as a group of models connected by a formal analogy [9]. In spite of the SOC being a controversial matter, that concept has a great heuristic value as a stimulating factor to create new ideas or construct models [11].

4 Implementation of Cellular Automata

We define, after Wolfram [28], cellular automata (CA) as a simple mathematical system which is able to exhibit complex behavior. The cellular automata according to von Neumann's idea, is defined as a system based, among others, on the following assumptions: homogenous structure of automata sited on regular net, finite number of states of each cell, the development of each cell defined by rules, state of all net changes synchronized. Automata structure depends on three parameters: dimension of space (n-dimensional grid), regularity condition (triangular, square or hexagonal cell) and number of neighbors (so-called von Neumann, Moore or Margolus neighborhood). The theory of cellular automata is extended to aspects of asynchronous work, graph automata with modify neighborhood, cellular automata with memory and other.

Cellular automata have vast applications that spread into almost every part of social life, including e.g. transport questions, percolation phenomena, or creation of social opinion [19,20].

The phase transition models mapping on cellular automata structure are based, in general, on model of magnetic phenomena. We could mention here, among others, Ising's model, *XY* model, Heisenberg's model, Gauss' model, or percolation model [4]. Models in the digital simulation process are supported by diverse methods and algorithms, including the Monte Carlo method and the Metropolis or Wolff algorithms.

In the first-order phase transition the first derivative of free energy f has discontinuity (as we consider above) what means that the process involves a latent heat. The emerging transport problems connected with high values of latent heat (liquid-vapor, liquid-solid etc. phase change) exclude application of Ising's model. The first-order phase transition model needs whole identification of creation of a new phase, what in our opinion is connected with nucleation process over structural defects and fluctuations within the interfacial layer. Reliable step towards the problem solution has been seen in the probabilistic switching rules [22]. A few models would be treated as a significant approximation of first-order phase transition within modeling physical process e.g. re-crystallization phenomena mapping on

cellular automata [32], modeling with applied Kauffman's Boolean networks [8], probabilistic cellular automata with memory [1], modeling on the microscopic level [33]. Application of the renormalization group method to description of that kind of phase change is improper because of lack of identifiable invariants within the scaling process [21].

The second-order phase transition (or continuous phase change) in magnetic or crystal structure is modeled with the renormalization group method, Ising's or Heisenberg's models and other. The several phase change phenomena in monocrystal structure are simulated by means of cellular automata e.g. Ising's model implemented on probabilistic cellular automata [7], application of the Creutz demon on cellular automata for description of phase change in EuTe - antiferromagnetic substance [13].

The phenomenological renormalization group method is applied to study critical properties of the Domany-Kinzel probabilistic cellular automata for description of continuous phase transition [2,24]. The dynamically driven renormalization group is used to probabilistic cellular automata having one absorbing state [34]. The application range of cellular automata continuously extends with reference its basic idea e.g. in the Domany-Kinzel, Kauffman, Rothman-Keller, Creutz demons and other models.

The dynamic SOC systems evolving to approach a critical point form new state of system in absence of any external pressures. The question referenced to application of the SOC models is connected with the criterion of falsifiability as defined by K. Popper. For several reasons the SOC does not seem to be a scientific theory, as we discuss above. If we accept the SOC as a sketch towards successfully research, it would be applied to modeling phase transition e.g. in absorbing-state referenced BTW dynamics model [6,9]. The SOC feature occurring is studied for realm of natural systems based on cellular automata (e.g forest fire [23], earthquake [19,25]), for abstractive realm [5,26,27] and many other.

5 Conclusions

The current studies on critical phenomena are characterized by creation universality and scaling hypothesis together with a deep conviction about a simple structure of the real world. That kind of belief is based on a possibility of modeling complex systems by adding simple and interactive elements (SOC, CA) or looking for universality features (RG). The first-order phase transition needs an operating interfacial layer model. The phenomenological approach would be effective if it will be possible to define universality hypothesis as it was done for the continuous phase change. The renormalization group method is inapplicable in that case and, moreover, it could not describe phenomena on the microscopic level.

Cellular automata, as we consider above, are based on several principles, among which the most important are: the finite number of states and the same rule of updating for each cell. As far as model interfacial layer within nucleation and heat transport processes are concerned, the problem becomes more complicated on the formal description level, so as the simulation process with cellular automata (microscopic approach without a transport process is cited above).

The phenomenological description of the continuous phase change is enabled with the renormalization group method and cellular automata as a simulation tool. The extremely interesting question in the continuous phase change, as we refer to the first-order phase transition, is variable description on the microscopic level. Furthermore, from the simulation point of view, cellular automata have restrictions similar to the problems in the interfacial layer analysis, but in the continuous case the microscopic description of enormous fluctuations near the critical point becomes too complex.

Within the last considered group of critical phenomena, a mapping of the SOC systems on cellular automata is applied. The long-term fluctuation problem is solved using the scaling method, a modification of boundary types or other methods. It seems that the fundamental problem in that kind of systems is a proof of existence of the SOC feature, which is possible to demonstrate in the numerical way only. The formal analogy applied in the latter case is insufficient for establishing a theory and for effective simulating. A promising step towards the SOC theory is the renormalization group method with cellular automata applied to problems of the SOC realm [30,31].

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