Cellular Automata Approach to Site Percolation on \mathbb{Z}^2 . A Numerical Study

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We present a cellular automata model as a new approach to Bernoulli site percolation on the square lattice. A new macroscopic quantity is defined and numerically computed at each level step of the automata dynamics. Its limit manifests a critical behavior at a value of the site occupancy probability quite close to those obtained for site percolation on \mathbb{Z}^2 with the best-known numerical methods.

KEY WORDS: Cellular automata; square lattice site (bond) percolation; fractal percolation.

1. INTRODUCTION

The concept of cellular automata (CA) was introduced in 1950⁽¹⁾ by von Neumann and Ulam as a system whose main feature was the ability to reproduce itself like a living organism. The well-known "game of life" proposed by J. Conway illustrates this biological aspect of CA and brought a renewal of attention to these models. The interest in the study of these complex systems stems from the fact that they demonstrate successful applications in natural sciences, in particular in hydrodynamics for various models of fluid flows.⁽²⁾ In this context, they are called "lattice gas cellular automata." In addition they are of great interest in computation theory, complexity analysis, and the study of critical phenomena in statistical physics.

Formally, cellular automata are dynamical systems where space, time, and state dynamical variables are discrete. Consider a *d*-dimensional lattice

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 \mathcal{L} , whose sites are called cells. $X \in \mathbb{Z}^d$ is the position of a given cell in \mathcal{L} . Each cell is assigned a state which is an integer from the set $\{0, 1, 2, ..., M-1\}$, where M is a natural number indicating the number of states. In the important class of "Boolean automata," the state variables belong to the set $\{0, 1\}$, in other words, sites are assigned a one-bit variable.

A neighborhood N of a cell c is a set of cells located at some distance δ from c. For example, a von Neumann neighborhood on the square lattice \mathbb{Z}^2 consists of all cells $X = (x, y) \in \mathbb{Z}^2$ at a distance one from the cell $X_0 = (x_0, y_0)$, such that $x = x_0$, $|y - y_0| = 1$ or $y = y_0$, $|x - x_0| = 1$. A Moore neighborhood involves the eight cells having one edge or one corner in common with the cell c.

The system evolves in discrete time steps according to a parallel dynamics described by a local rule which updates the state of each cell according to the state of all other cells in its neighborhood. If $x_{i,j}^t$ is the state variable at time t assigned to the cell at position $X_{i,j}$, then in the case of a von Neumann neighborhood, the state of this cell at time t + 1 is given by

$$x_{i,j}^{t+1} = f(x_{i-1,j}^{t}, x_{i+1,j}^{t}, x_{i,j-1}^{t}, x_{i,j+1}^{t})$$

where f is the local updating function (also called transition rule of the CA). This synchronous updating defines a global function defined on the set of all cell configurations on \mathcal{L} .

The long-time behavior of CA dynamics, described by the global function, has been investigated by Wolfram,⁽³⁾ who attempted a classification of all possible CA into four classes, today named after him:

Class I: CA dynamics evolves toward a constant state which is a fixed point of the synchronous dynamics.

Class II: CA dynamics evolves toward periodic configurations.

Class III: Evolution toward fully chaotic states.

Class IV: Evolution toward a quiescent state comprising localized bounded chaotic states.

Wolfram also established a well-accepted notation for CA rules. A (k, r) rule stands for a *k*-states linear CA (for which the local rule is linear with respect to the states of the cells in the neighborhood N) and r represents the number of involved neighbors. As we shall see later, the CA considered in this note seems to belong to Wolfram's class I.

Applications of CA in statistical physics reveal promising aspects and at the same time difficult mathematical problems to solve. Equivalence between Ising models and directed percolation problems with CA has been proven by Domany and Kinzel.⁽⁴⁾ In this paper we present a model

CA Approach to Site Percolation

of CA that seems to be related to the critical behavior of the square site percolation problem on \mathbb{Z}^2 . The next section gives a short account of percolation problems and some recent results in the field. In Section 3 we introduce a cellular automaton defined on the square lattice \mathbb{Z}^2 . Its dynamics shows a critical behavior for a value of the site probability which seems to be related to the numerically estimated threshold probability for site percolation on \mathbb{Z}^2 . Section 4 is devoted to some remarks.

2. A SHORT REVIEW ON PERCOLATION

The problem of percolation was posed in 1957 by Broadbent and Hammersley⁽⁵⁾ in the following terms. We are given a large porous stone in a bucket of water: is the center of the stone wetted or not? In other words, does the water percolate through the stone? Percolation models were also considered in connection with spread of disease through populations, e.g., in orchards.

Typically one formulates a simple stochastic model for such a situation which in two dimensions can be described in the following way. Let $p \in [0, 1]$ and consider the square lattice \mathbb{Z}^2 . The edges of the lattice are assigned at random and independently of each other the probability p of being open and the probability 1 - p of being closed. For the infinite lattice \mathbb{Z}^2 this assignment is equivalent to removing a fraction 1 - p of all edges at random. Two vertices are called connected if there exists at least one path between them consisting solely of open edges. The edges of \mathbb{Z}^2 represent the passage ways of the stone and p is the proportion of passages which are broad enough (open) to allow water to pass along them. This model is known as independent (Bernoulli) edge (or bond) percolation. For a nice general review we refer to Grimmett⁽⁶⁾ and the references therein.

For the independent (Bernoulli) site percolation model on \mathbb{Z}^2 , we also fix a probability $p \in [0, 1]$. We again turn \mathbb{Z}^2 into a graph, denoted by \mathbb{L}^2 , by adding edges between all pairs of vertices of \mathbb{Z}^2 which are at distance one from each other, i.e., all pairs (x_1, x_2) , (y_1, y_2) of vertices of \mathbb{Z}^2 such that $x_1 = x_2$, $|y_1 - y_2| = 1$ or $y_1 = y_2$, $|x_1 - x_2| = 1$. We examine now each site of \mathbb{L}^2 : with probability p the sites of \mathbb{Z}^2 are occupied, and with probability 1 - p they are vacant. We delete all bonds having a vacant site as an endpoint, independently of all other sites.

For p = 0 the resulting graph consists only of isolated sites, while setting p = 1 yields the whole original graph \mathbb{L}^2 , which consists of one unbounded component, namely itself. If p is small, one sees a lot of isolated clusters, each consisting of interconnected occupied sites and surrounded by a sea of vacant sites. As p increases, it reaches a critical value p_c above which there

appears with positive probability an unbounded component in the resulting graph. Physically speaking the question is whether or not there exists a nontrivial phase transition with respect to the connectivity properties of the system.

Although the above models are very easy to describe, they prove hard to solve. A full mathematical solution is still lacking and presents a great challenge. For independent percolation on \mathbb{L}^d only one critical value is known. Indeed Kesten^(7,8) showed that $p_c^{\text{bond}}(\mathbb{Z}^2) = 1/2$. This result is far from trivial and such an exact calculation does not exist for the two-dimensional site problem. The best rigorous available bounds on the site critical percolation probability in \mathbb{L}^2 are $0.543 \leq p_c^{\text{site}}(\mathbb{Z}^2) \leq 3/4$. The first inequality is due to Men'shikov and Pelikh⁽⁹⁾ and the second one was already derived by Broadbent and Hammersley.⁽⁵⁾ These bounds are still far from the threshold value obtained by computer simulations, which is around 0.59.⁽¹³⁻¹⁶⁾

It is well known that every bond model can be reformulated as a site model, but that the converse is false.⁽¹⁰⁾ In other words, site percolation models are more general than bond percolation models (see ref. 8, Chapter 3). Consider bond percolation on a lattice \mathscr{L} . The covering lattice \mathscr{L}_c of \mathscr{L} is defined in the following way. To each edge of \mathscr{L} there corresponds a vertex of \mathscr{L}_c and two such vertices are called adjacent in \mathscr{L}_c if and only if the corresponding edges of \mathscr{L} have an end vertex in common. Therefore it is indeed exactly equivalent to study bond percolation on \mathscr{L} and site percolation on the covering lattice \mathscr{L}_c .

There is also a nice connection between Mandelbrot's fractal percolation process⁽¹¹⁾ and independent site percolation on \mathbb{Z}^2 . Mandelbrot's fractal percolation process can be described as follows. Fix an integer $N \ge 2$ and $p \in [0, 1]$. We divide the unit square $[0, 1] \times [0, 1]$ into N^2 smaller squares of size $1/N \times 1/N$ and each of these subsquares is retained with probability p and deleted with probability 1-p. Let us call M_1 the retained set. We now repeat this process in each of the squares of M_1 : each subsquare of M_1 is divided now into N^2 smaller squares of size $1/N^2 \times 1/N^2$ and each of these smaller subsquares is again retained with probability p and deleted with probability 1-p. The retained set is denoted by M_2 . After N iterations we obtain the retained set M_N and in this way a sequence of decreasing random sets $M_1, M_2, ..., M_N$. We now define M_{∞} by

$$M_{\infty} = \bigcap_{N=1}^{\infty} M_N \tag{2.1}$$

and percolation occurs if M_{∞} contains a connected component which intersects the bottom and the top of the unit square. The threshold value

CA Approach to Site Percolation

of p is called $p_{c,N}$. For N very large the system looks indeed like independent site percolation on the square lattice \mathbb{Z}^2 if we view the squares as sites in \mathbb{Z}^2 . Mandelbrot⁽¹¹⁾ has proposed the conjecture that

$$\lim_{N \to \infty} p_{c,N} = p_c^{\text{site}}(\mathbb{Z}^2)$$
(2.2)

This conjecture was proved in 1989 by Chayes and Chayes.⁽¹²⁾

At the percolation transition the cluster distribution is scale invariant, as can be demonstrated by comparing a typical configuration at p_c with a magnified portion of itself. In this paper we report the results of numerical simulations concerning an alternative approach, based on a scaling technique to the site percolation problem on \mathbb{Z}^2 . A mathematical study of the method we propose is deferred to another publication.

3. THE MODEL

For $n \in \mathbb{N}$, consider an $n \times n$ lattice $\mathbb{L}_n^2 \subset \mathbb{Z}^2$ with free boundary conditions. For $p \in [0, 1]$ build a site configuration $\sigma(\mathbb{L}_n^2)$ in the following way: go through all sites $(i, j) \in \mathbb{L}_n^2$ and for each site, put a 1 with probability p and a 0 with probability 1 - p, independent of all other sites.

Call S_i the *i*th line vector of 0–1 digits in $\sigma(\mathbb{L}^2_n)$, $S_i \in \{0, 1\}^n$. For any site configuration $\sigma(\mathbb{L}^2_n)$, let us define the mean local overlap (see Fig. 1)

$$\Pi(n, p) = \frac{1}{n^2} \sum_{i=1}^{n} \langle S_i, S_{i+1} \rangle$$
(3.1)

where $\langle \cdot, \cdot \rangle$ is the usual scalar product in $\{0, 1\}^n$; namely

$$\langle S_i, S_{i+1} \rangle = \sum_{j=1}^n S_i^j \cdot S_{i+1}^j, \qquad S_k^j \in \{0, 1\}$$
 (3.2)

It is easy to see that $\lim_{n \to \infty} \Pi(n, p) = p^2$, since $S_i^j \cdot S_{i+1}^j = 1$ if and only if $S_i^j = 1$ and $S_{i+1}^j = 1$, and this event has probability p^2 .

Actually the function $\Pi(n, p)$ contains information related to the bottom-to-top connectivity of occupied sites, but if we want to view

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	0	1	1	0	1	0	0	0	1	0	0	0	1	0	1	0	1	1	
	1	1	0	1	1	0	1	0	1	0	1	1	1	0	0	1	0	0	$-S_{i+1}$
	0	1	1	0	1	0	1	0	0	1	0	1	0	1	0	0	1	1	← S;
_	1	0	1	0	0	1	0	1	1	0	0	1	0	1	1	0	0	1	

Fig. 1. Part of $n \times n$ lattice, with line vectors of sites $S_i \in \{0, 1\}^n$.



Fig. 2. Isolated cluster of occupied sites contributing to $\Pi(n, p)$.

 $\Pi(n, p)$ as an appropriate quantity describing the critical behavior of the cluster size distribution near p_c , it counts too much! For example, the configuration of Fig. 2 will contribute to $\Pi(n, p)$ though it will not contribute to long-range percolation.

The idea we propose is to rescale $\sigma(\mathbb{L}_n^2)$ in order to retain only the information related with long-range percolation, and get rid of patterns like the one in Fig. 2.

We consider 2×2 cells on the grid. The following Boolean automaton rule has been applied since it preserves locally (i.e., on the level of the elementary cells) the connectivity from bottom to top:

$$(S_{i}^{j})^{(t+1)} = \left[(S_{i}^{j})^{(t)} \land (S_{i+1}^{j})^{(t)} \right] \lor \left[(S_{i}^{j+1})^{(t)} \land (S_{i+1}^{j+1})^{(t)} \right]$$
(3.3)

In this way each elementary 2×2 cell is replaced by a new "supersite," which represents the mean (in the sense of our rule) of the four initial sites.

A distinguished feature here is that the automaton rule is applied with overlapping cells all over the lattice with free boundary conditions as seen in Fig. 3.

The procedure has been simulated on a CM2 connection machine for a 4096×4096 lattice and thousands of time steps of synchronous automaton dynamics starting from a randomly chosen initial configuration with

 1	1	0	1	0	0	1	1	0	1	0	0	0	1	0	
0	0	1	0	1	1	1	0	0	1	0	1	1	0	0	
0	1	1	0	0	1	0	0	1	0	1	0	0	1	0	
1	1	0	1	1	0	1	1	0	0	0	1	0	1	1	_

Fig. 3. Cells neighborhood considered in this automaton rule. The updated cell is the bottom leftmost cell of each 2×2 cell pattern.



Fig. 4. $\Pi(n, p)$ as a function of p on a square site lattice with linear size n = 4096 for different timesteps of the synchronous dynamics.



Fig. 5. Limiting behavior of the "S-like" shape of $\Pi(n, p)$ showing a transition close to p = 0.593.

a given initial site probability p. From accurate statistics on the limiting behavior of CA dynamics, we find that $\Pi(n, p)$ shows a sharp transition in the topological structure of the random lattice at $p_0 = 0.593 \pm 0.001$.

Figure 4 shows the evolution of $\Pi(n, p)$ as a function of p for n = 4096 and several steps of dynamics and Fig. 5 shows the corresponding limiting behavior.

Gebele⁽¹⁵⁾ has found the following numerical estimate for the critical probability for site percolation on \mathbb{Z}^2 : $p_c = 0.5927 \pm 0.00005$. Derrida and Saleur⁽¹⁶⁾ showed by using Monte Carlo and transfer matrix methods that $p_c = 0.592 \pm 0.0015$.

We want to point out that one does not need to consider large cell neighborhoods in order to get close to the estimated value of p_c , as done in ref. 13, for example. There, in order to get close enough to p_c , the elementary cell size had to be increased by factors up to few hundred.

4. FINAL REMARKS

Let us briefly discuss our future plans and point out some open questions that have not been discussed in this paper but appear to us as quite interesting.

1. Numerics: We intend to perform larger and more accurate numerical computations in order to refine our estimate of p_0 .

2. Theory: The question of how the automaton rule acts in the large is far from being trivial:

(a) There exist locally percolating patterns $(k \times k \text{ patterns showing a crossing of 1 from bottom to top) that are distroyed by the rule <math>(k-1 \text{ automaton steps acting on this original pattern end with a 0 supersite)}$ (Fig. 6).

(b) The reverse is also true; there exist locally nonpercolating patterns giving rise to an occupied 1 supersite.



Fig. 6. Example showing that the automaton rule may violates locally the connectedness of occupied clusters.

CA Approach to Site Percolation

Nevertheless, the results of the computer simulations seem to indicate that in the limit, the pathological configurations do not contribute to the function $\Pi(n, p)$ controlling the mean overlap.

Indeed, numerical experiments made on small $(k \times k)$ cells show that these events have indeed negligible weight (for k = 4 or 5 the fraction of these events is about 10^{-3} when compared to locally percolating patterns giving 1 after application of the global automaton dynamics).

One way to prove that our model gives the correct answer to the problem of site percolation on \mathbb{Z}^2 would be to connect it to a fractal percolation problem as defined in ref. 11 and investigated in refs. 12 and 17, for example, and to show that the two problems are in some sense probabilistically equivalent to each other.

The hard part comes from the fact that the rule being used does not leave invariant an important class of events (increasing events) on $\sigma(\mathbb{L}^2_n)$, for which there exist many useful results to work with (Harris-FKG and BK inequalities, Russo's formula, etc.^(6,8)).

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