CELLULAR AUTOMATA MODELS OF RING DYNAMICS

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This paper describes three models arising from the theory of excitable media, whose primary visual feature are expanding rings of excitation. Rigorous mathematical results and experimental/computational issues are both addressed. We start with the much–studied *Greenberg–Hastings model (GHM)* in which the rings are very short–lived, but they do have a transient percolation property. By contrast, in the model we call *annihilating nested rings (ANR)*, excitation centers only gradually lose strength, i.e. each time they become inactive (and then stay so forever) with a fixed probability; we show how the long–term global connectivity properties of the set of excited sites undergo a phase transition. Second part of the paper is devoted to *digital boiling (DB)* in which new rings spontaneously appear at rested sites with a positive probability. We focus on such (related) issues as convergence to equilibrium, equilibrium excitation level and success of the basic coupling.

Keywords: correlation length, coupling, excitable media, Greenberg–Hastings model, percolation.

1. Introduction

Rings are a primary visual feature of many natural processes, and arise in many simple mathematical models amenable to computer experimentation. Ring dynamics have thus frequently appeared in the applied literature, in which they are often referred to as *target states*. They have been observed in a variety of biological and chemical processes, arguably the most famous of which is the Belousov–Zhabotinsky reaction. Many more instances of ring dynamics are described in the special issue of Physica D 49 (1991), titled *Waves and patterns in chemical and biological media*). Other recent examples include convection patterns[1] and a model which obtains spiral and circular waves by emulating the moiré effect[19].

Our interest in phenomena associated with ring dynamics arose from studying a simple cellular automaton model for two–dimensional excitable media, called the *Greenberg–Hastings model (GHM)*[7,8]. Originally introduced in Refs. 23 and 15, this model, and its relatives, has been studied by a number of researchers from various fields (see Refs. 3–5, 7–9, 17, 20, 22 and many

further references contained in these papers). In particular, study of ring dynamics in the GHM was initiated in Ref. 9; in deference to this pioneering paper we keep its basic set–up, which we describe next.

All models described in this paper live on two–dimensional square lattice $\mathbf{Z}^2$. We will assume that the *neighborhood* $\mathcal{N}_x$ of a site $x \in \mathbf{Z}^2$ consists of the nearest 8 points (usually called the *range 1 box* or *Moore* neighborhood). This assumption is merely for concreteness; all described results remain true in greater generality[12]. For the basic GHM, every site $x \in \mathbf{Z}^2$ is in one of three states: the rested state 0, the excited state 1, or the refractory (or recovering) state 2. The discrete time update rule stipulates that every 1 changes into 2 automatically, and so does every 2 into 0. However, a 0 at x will change into a 1 if and only if a 1 is present in $\mathcal{N}_x$. Formally, if $\gamma_t(x)$ denotes the state of site x at time t, then

$$\gamma_{t+1}(x) = \begin{cases} 2, & \text{if } \gamma_t(x) = 1, \\ 1, & \text{if } \gamma_t(x) = 0 \text{ and } \mathcal{N}_x \text{ contains a } y \text{ with } \gamma_t(y) = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{1.1}$$

Hence the the entire evolution is determined as soon as the initial state γ_0 is specified. As Fraser and Kapral have observed in Ref. 9, started from an initial positive density of 1's on a background of 0's, the rule (1.1) generates short–lived square rings of excitation which however can form infinite connected sets in a very narrow window of time. We will make a more precise statement on this below, for now we refer the reader to Ref. 10 for an illustration of this phenomenon by a computer simulation.

To overcome this lack of recurrence in a convenient fashion, we introduce external stimulation into the basic GHM given by (1.1). We propose a rule with two probabilities $p_f, p_s \in [0,1]$, which envisions every site $x \in \mathbf{Z}^2$ either in one of the ordinary states 0,1,2 or in one of the externally excited states e_0, e_1, e_2. The externally excited states behave as "pacemakers": they go through their excitation cycle automatically. However, they turn into ordinary states with probability $1 - p_f$ every excitation period. The three normal states behave as in (1.1). Finally, we incorporate continuous nucleation by declaring that a 0 may spontaneously turn into a new externally excited site e_1 with probability p_s. To be more precise, we define the *externally stimulated GHM (ESGHM)* $\tilde{\gamma}_t$ by the following transition rule at a site $x \in \mathbf{Z}^2$:

$$\left.\begin{array}{l} 1 \to 2 \\ 2 \to 0 \\ e_0 \to e_1 \\ e_2 \to e_0 \end{array}\right\} \text{ automatically,}$$

$$\begin{array}{ll} e_1 \to e_2 & \text{with probability } p_f, \\ e_1 \to 2 & \text{with probability } 1 - p_f, \\ 0 \to 1 & \text{if there is either a 1 or an } e_1 \text{ in } \mathcal{N}_x, \\ 0 \to e_1 & \text{with probability } p_s, \text{ if } \mathcal{N}_x \text{ contains no 1 or } e_1, \\ 0 \to 0 & \text{with probability } 1 - p_s, \text{ if } \mathcal{N}_x \text{ contains no 1 or } e_1. \end{array} \tag{1.2}$$

We will address the long–term behavior of the ESGHM in two extreme cases, when either p_f or p_s is 0. Firstly, we assume that $p_s = 0$ and that $p_f \in (0,1)$. Start with a single e_1 surrounded by 0's. This e_1 proceeds to generate a geometrically distributed number of concentric expanding square rings before it finally turns into a 2. The created nested rings then keep expanding forever. If we start with two e_1's, rings of the same size annihilate upon collision along their intersection. For this reason, we refer to the dynamics in this regime as the *annihilating nested rings (ANR)*. As we will describe in more detail Section 2, connectivity properties of the set of 1's undergo a curious phase transition as p_f changes from 0 to 1. If p_f is small, the set of 1's oscillates between forming infinite connected sets and being very far from doing so. By contrast, if p_f is close to 1, the set of 1's is always close to large scale connectivity.

Suppose now that $p_f = 0$, $p_s > 0$, and therefore identify e_1 with 1. Visual features of this dynamics resemble bubble formation, growth and annihilation in a boiling liquid (see Figure 2 or Feb. 12, 1996 Recipe of Ref. 17), hence we call this case of the ESGHM *digital boiling (DB)*.

Although it arises naturally from excitable media modeling, there is another reason why the DB is of interest to us. Namely, the creation/annihilation dynamics of DB resembles main features of simplest difference processes for growing connected interfaces in three dimensions. Indeed, we now construct a growing interface dynamics for which the 1's in DB represent *exactly* the contour lines of same height (that is, they have the same meaning as the contour lines of a relief map). Assume that the description of the interface $\tilde{\xi}_t$ is given by its positive integer height above every site $x \in \mathbf{Z}^2$; hence $\tilde{\xi}_t(x) = k$ means that the height of the interface above the site x is k. The following rule then determines how this interface grows:

(I1) If there is at least one $y \in \mathcal{N}_x$ with $\tilde{\xi}_t(y) > \tilde{\xi}_t(x)$, then $\tilde{\xi}_t(x)$ advances automatically by 1.

(I2) Otherwise, if $\tilde{\xi}_t(x) = \tilde{\xi}_{t-1}(x) = \tilde{\xi}_{t-2}(x)$, then $\tilde{\xi}_t(x)$ advances by 1 with probability p_s.

(I3) In other cases $\tilde{\xi}_t(x)$ stays the same.

Denote by $N_t(x)$ the number of times x is excited in the DB dynamics during the time interval $[0,t]$. Then it is not hard to see that, under the natural coupling between the two processes, $N_t(x) = \tilde{\xi}(x)$. (Hence the awkward condition (I2) involving the previous two times stems from the fact that only 0's can be externally excited in the DB.) Various dynamics similar to the one given by the update rule (I1)–(I3) have appeared in the literature. For example, a closely related continuous–time version was analyzed in Ref. 18 . Another relative of (I1)–(I3) is the synchronization dynamics described in Section 9.6 of Ref. 21, and discussed in Refs. 16 and 6. The basic coupling method from Ref. 6 can be used to analyze the one–dimensional version of DB dynamics, whereas, as we will see in Section 3, the corresponding coupling in two dimensions is much more elusive. Thus the uniqueness of invariant measure and convergence to equilibrium remain open problems on the rigorous level. It is, however, possible to prove a strong law for $N_t(x)$ and estimate the order of the resulting time constant.

In conclusion, we briefly discuss limitations and possible generalizations of models discussed here. We should start by mentioning that our approach depends crucially on synchronicity; the evolution of an asynchronous GHM–type system will not be dominated by rings, but will either die out or approach a spiral equilibrium[4,8]. Another possible generalization involves threshold–range GHM, in which a 0 will change into a 1 only if number of 1's in its (perhaps rather large) neighborhood exceeds a prescribed threshold[7]. Even survival of rings from deterministic finite configurations of 1's becomes a difficult issue in this case [11]. Moreover, we suspect that, started from random initial seeds of excited states, debris left from failed nuclei is able to break the rings, resulting in most cases in local periodicity or relaxation (Ref. 7 contains definitions and some discussion on these issues). Finally, we should mention that all discussed models make sense in higher dimensions, and some aspects of them can be studied using techniques from Ref. 12; of course, computational problems become much more difficult.

In the remainder of the paper, we give a more detailed account on rigorously known results and some findings suggested by simulations. We leave out the detailed proofs, which will appear in Refs. 10 and 12. As the reader will see, many issues remain unclear even on the experimental level; however, perhaps a more powerful computation environment would suffice for the resolution of some of these problems.

2. Evolution of connectivity in the GHM and the ANR

We start with a definition, that will tell us how far a set $A \subset \mathbf{Z}^2$ is from including an infinite connected set. The idea is quite natural and simple: measure the smallest upper bound on jump size which will still enable one to hop to infinity on sites of A. To be more precise, fix a finite set $\mathcal{D} \subset \mathbf{Z}^2$ and say that A *$\mathcal{D}$–percolates* if there exists an infinite sequence $x_1, x_2, \ldots$ of distinct sites in A such that $x_{k+1} - x_k \in \mathcal{D}$ for $k = 1, 2, \ldots$. We will only use boxes $B_\infty(0,R) = \{(x,y) : |x| \le R, |y| \le R\}$ for the set $\mathcal{D}$; in particular, if the set A $B_\infty(0,1)$–percolates, then in the usual terminology it *ℓ^∞–percolates*. Exactly how far A is from ℓ^∞–percolation is then measured by

$$PercFail(A) = \sup\{a : A \text{ does not } B_\infty(0, a+1)\text{–percolate}\}.$$

Loosely stated, then, the set A percolates if jumps of sizes up to $PercFail(A) + 1$ are allowed, while it does not if only jumps of sizes at most $PercFail(A)$ are permitted.

We start by describing the percolation properties of the set of excited sites in the GHM. Most of the theorem below is discussed in considerable detail in Ref. 10, with the exception of (3), which can be proved by a simple rescaling argument.

Theorem 1. *Assume that the initial state γ_0 of the GHM is the product measure with a fixed density $p > 0$ of 1's on a background of 0's, that is, $P(\gamma_0(x) = 1) = 1 - P(\gamma_0(x) = 0) = p$.*

(1) Each site x has a unique time t at which $\gamma_t(x) = 1$.

(2) For each p there exists a time $T(p)$ such that the set $\{\gamma_t = 1\}$ of excited sites at time t ℓ^∞–percolates for $t = T(p)$, but does not ℓ^∞–percolate either for $t < T(p)$ or for $t > T(p) + 1$. As $p \to 0$, $T(p)\sqrt{p}$ converges to a positive finite constant.

(3) As t increases to ∞, PercFail$(\{\gamma_t = 1\})$ increases exponentially in t^2, more precisely, $t^{-2} \log$ PercFail$(\{\gamma_t = 1\}) \to -4\log(1-p)$.

Therefore, the excited sites in the GHM ℓ^∞–percolate for at most two time units at about time constant$\cdot p^{-1/2}$, then quickly get very far from percolation. One should not expect this to happen in the ANR model, in particular it is easy to see that every site must get excited infinitely many times. Indeed, the following rigorous result was proved in Ref. 12.

Theorem 2. *Assume that the ANR $\tilde{\gamma}_t$ is started from the fully excited state $\tilde{\gamma}_0 \equiv e_1$.*

(1) The density of 1's $P(\tilde{\gamma}_t(x) = 1)$ decays as $1/t$, that is, there exist two finite non–zero constants $C_1 = C_1(p_f)$ and $C_2 = C_2(p_f)$ such that for $t > 0$

$$\frac{C_1}{t} \le P(\tilde{\gamma}_t(x) = 1) \le \frac{C_2}{t}$$

(2) With probability 1, the set of excited sites $\{\tilde{\gamma}_t = 1\}$ ℓ^∞–percolates infinitely many times, and fails to ℓ^∞–percolate infinitely many times.

(3) There are constants $0 < \mu_{lc} \le \mu_{uc} < 1$, such that $p_f < \mu_{lc}$ implies

$$\limsup_{t\to\infty} \frac{\mathit{PercFail}(\{\tilde{\gamma}_t = 1\})}{t}$$

is a non–zero finite number with probability 1. On the other hand, if $p_f > \mu_{uc}$ then

$$\limsup_{t\to\infty} \mathit{PercFail}(\{\tilde{\gamma}_t = 1\})$$

is a finite non–zero number with probability 1.

While (1) guarantees that the density of excited sites decays for any p_f, (2) and (3) show that connectivity properties of this set undergo a phase transition as p_f changes from 0 to 1. For large p_f, the set of 1's never gets very far from percolation; however, at large times one has to go quite far from the origin before one encounters the infinite "almost connected" set. On the other hand, for small p_f, the set of 1's occasionally gets to be a constant$\cdot t$ away from forming connected set, although it always bounces back to ℓ^∞–percolation.

We should mention that while the constants C_1 and C_2 from Theorem 2(1) cannot be made equal, it is conjectured that the phase transition described in (3) is sharp, i.e. that μ_{lc} and

μ_{uc} are equal to a common critical probability μ_c. Lack of appropriate continuum percolation technology makes this exceedingly difficult to prove rigorously. The reader is referred to Ref. 12 for more details on this thorny issue.

Figure 1 illustrates the ANR dynamics in the two regimes described in Theorem 2. Simulations are done on 400×400 boxes with periodic boundary conditions, excited sites are painted black, and refractory light gray (barely visible in the pictures). The left frame captures the state of the system with $p_f = 0.2$ at $t = 18$, while $p_f = 0.5$ and $t = 42$ in the right frame. (The two times are chosen to facilitate fair comparison: the expected number of externally excited sites in the square is close to 10 in both cases.) Note that the black pixels in the left frame are divided into small widely separated connected clusters, while they form connections which span the entire length of the square in the right frame. Although it is sometimes a little tricky to decide whether a particular p_f is above or below μ_c, we would, based on such simulations, expect that μ_c is somewhere between 0.3 and 0.35.

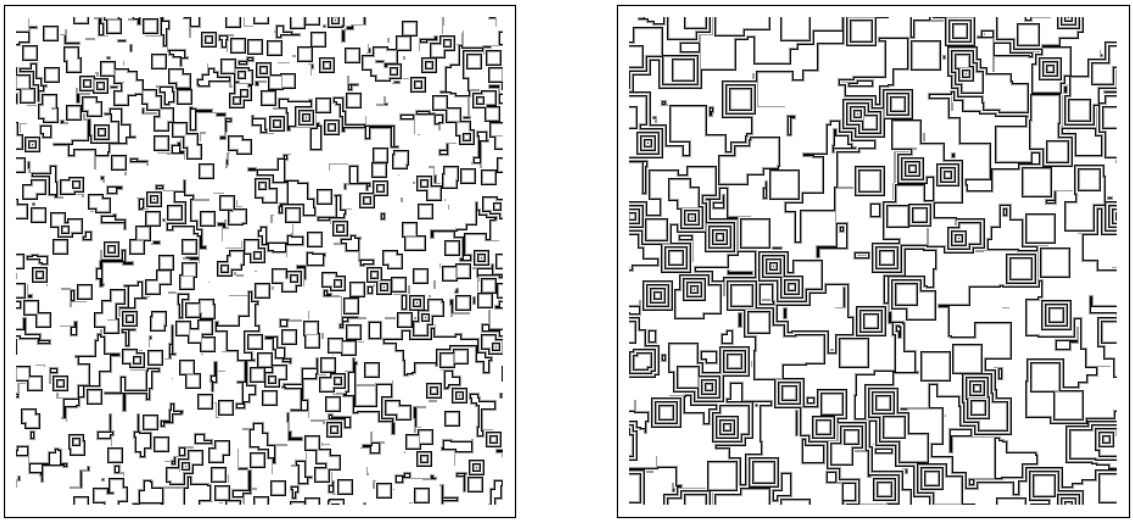

Figure 1. Two regimes of the ANR dynamics.

2. Ergodic behavior of the DB dynamics

As usual, we start with a rigorous result proved in Ref. 12. Recall that $N_t(x)$ simply counts the number of times $s \in [0, t]$ at which $\tilde{\gamma}_s(x) = 1$.

Theorem 3. *Assume that the DB dynamics $\tilde{\gamma}_t$ starts from the quiescent state $\tilde{\gamma}_0 \equiv 0$.*

(1) For every fixed p_s, $\frac{N_t(0)}{t}$ converges with probability 1 to a constant $\nu(p_s) \in (0, 1/3)$ as $t \to \infty$.

(2) $\nu(p_s)p_s^{-1/3} \to \nu^* \in (0,\infty)$ *as* $p_s \to 0$.

Therefore, a typical site gets excited about once every $1/(\nu^* p_s^{1/3})$ time steps. This strongly suggests that the system globally approaches a unique equilibrium which has density of excited sites about $\nu^* p_s^{1/3}$. However, it does not seem clear how to prove this result rigorously. Hence we resorted to computer experiments to gather some more evidence of its validity.

All our simulations were done on 400×400 boxes with periodic boundary condition, and we have fixed $p_s = 0.01$. The left side of Figure 2 shows the state of one such simulation at time $t = 2000$. The right side of the same figure shows how the density of 1's evolves during the first 200 time steps (the horizontal axis is time, and the vertical axis the average number of 1's per site). The system apparently undergoes deterministic damped oscillations up until about time 100, then it reaches an equilibrium. However, substantial equilibrium fluctuations of average density can be observed. Their amplitude goes down with the system size, as expected from the conjectured convergence to a unique invariant measure; however, the fact that they are so prominent on a relatively large array suggests possibly quite large equilibrium correlation length, corresponding to relatively large regions where density is either higher or lower than the average.

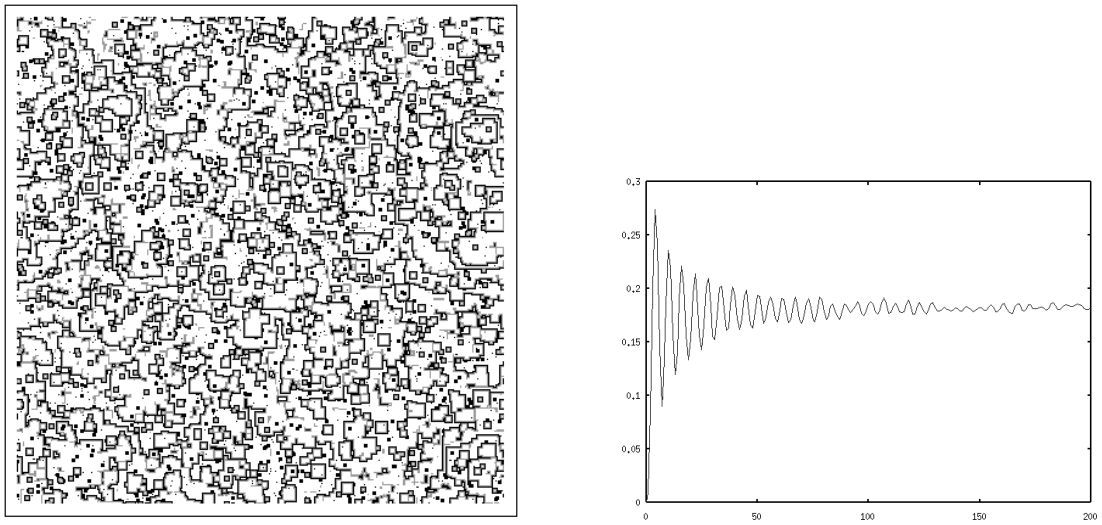

Figure 2. Equilibrium state and evolution of density for the DB dynamics.

The said fluctuations also make estimation of ν^* quite a demanding computational project. The convergence in Theorem 3 (2) seems to be quite slow and for small p_s one needs huge arrays to even make the regression analysis give a reasonable estimate for the correct exponent 1/3;

nevertheless, the statistical data suggest that ν^* is somewhere in the neighborhood of 1.3 (it can be proved rigorously that $\nu^* \in (0.75, 2.3)$).

One of the basic methods to simultaneously prove uniqueness of invariant measures and convergence is coupling. In the present context, one would have to show that it is possible to couple two systems started from different initial states so that the probability that they differ at any given site goes to 0 as time progresses. One immediate problem is that the allowed class of initial states must be very carefully restricted to those that include only rings, but we will skip over this theoretical issue. The most basic coupling is of course the one which uses the same coin flips (with probability p_s of heads) at every site and every time for both systems. This is how this coupling works: fix a time t and a site x, and flip the coin. If the outcome is tails, then apply rule (1.1); otherwise, change state of x at the next time to 1 for any system in which x is in state 0 at time t.

Recent methods of Eckhaus and Gray[6] can be utilized to show that the coupling described above is successful for nearest–neighbor DB in one dimension. Here we describe one experiment which enables us to at least speculate about the properties of this coupling in two dimensions.

In essence, we measure the effect a single extra step of the rule at the beginning has on state of the system at large times. That is, we couple two DB systems: $\tilde{\gamma}_t^{(1)}$ started at $\tilde{\gamma}_0^{(1)} \equiv 0$ and $\tilde{\gamma}_t^{(2)}$ whose initial set $\tilde{\gamma}_0^{(2)}$ has density p_s of 1's on the background of 0's. Then we record the evolution of density of disagreeing sites, i.e. sites x such that $\tilde{\gamma}_t^{(1)}(x) \neq \tilde{\gamma}_t^{(2)}(x)$.

In the physics literature, such coupling experiments are called *damage spreading* (or *damage healing*) and the resulting decay laws have been investigated theoretically and experimentally. An interesting recent example is Ref. 14 in which this method is successfully applied to Ising models.

Figure 3 includes a state of the systems at time 200 (this time, the sites which are painted black are those at which the two systems disagree, while light gray are 1's and 2's in the two systems). One observes that that the disagreeing sites form an annihilating ring system in which rings cannot be created away from existing ones; however, a ring in this system may expand at certain places and contract at others, therefore it can be pinched and become two or more rings. Thus the disagreeing sites form a kind of annihilating branching process and it not clear that their density converges to 0. Unfortunately, experimental evidence is also inconclusive; the right part of Figure 3 shows the evolution of density of these sites up to time 5000.

Once the coupled DB systems have reached equilibrium, rings of disagreeing sites are locally equally likely to move in any direction. This, as well as Figure 3, suggest that the rings in this system behave in a similar way as the boundaries between clusters in the stepping stone model[2];

however, substantial (but exponentially decaying) space and time correlations in the DB model should make the make the rings much less rugged. Thus a natural conjecture would be that their density goes to 0 as $t \to \infty$, albeit very slowly: perhaps like constant$\cdot(\log t)^{-1}$.

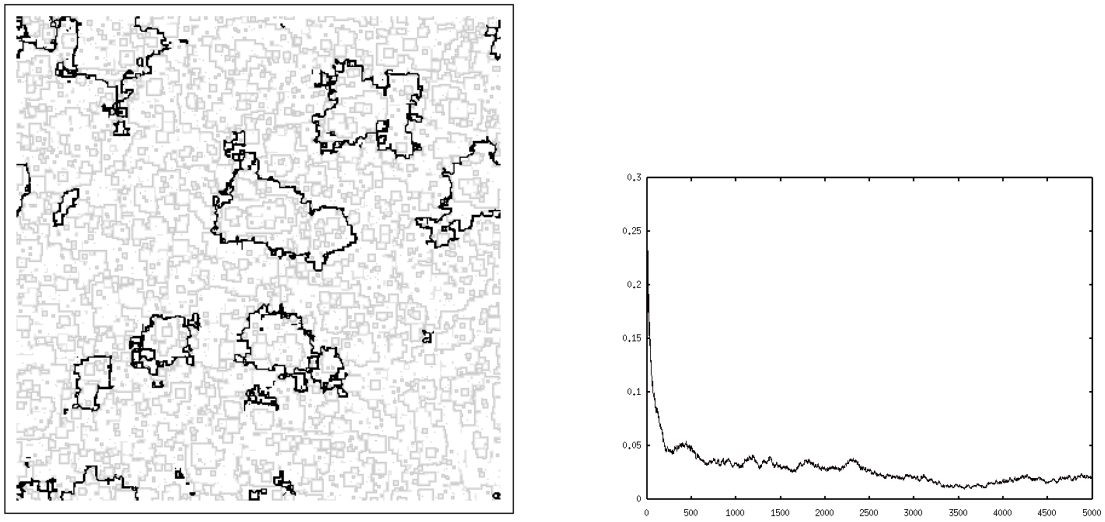

Figure 3. State of the coupling at time $t = 200$ and evolution of density of disagreeing sites.

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