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# Modeling nonequilibrium phase transitions and critical behavior in complex systems

J. Marro *, J.M. Cortes, P.I. Hurtado

*Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071-Granada, Spain*

**Abstract**

We comment on some recent, yet unpublished results concerning instabilities in complex systems and their applications. In particular, we briefly describe main observations during extensive computer simulations of two lattice nonequilibrium models. One exhibits robust and efficient processes of pattern recognition under synaptic coherent activity; the second example exhibits interesting critical behavior and simulates nucleation and spinodal decomposition processes in driven fluids. © 2002 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

Nature may be viewed as a collection of *complex systems* [1]. Consequently, a principal question is how these systems, which typically consist of many simple interacting units, develop qualitatively new and high-level kinds of organization. This is the problem of connecting the microscopics of constituents with the coherent structures that characterize organisms and communities. It may often be assumed that the fundamental laws of physics, such as Hamilton and Maxwell equations, are individual properties of the units. Still, it is only very rare that the origin and form of natural phenomena can be inferred from basic laws. What is the relevance of fundamental physics to predict the weather, to design new materials and drugs or to understand the origin of life? It is remarkable that statistical physics recently addressed the problem of connecting emergent behavior to the constituents' properties in a more indirect manner, too. That is, main concepts in the theory of phase transitions, such as correlations, criticality, scale invariance and self-similarity that characterize the global behavior of the simplest model cases happen to be ubiquitous in nature. This brings many interesting, high-level phenomena to the attention of physicists, and the study of (nonequilibrium) phase transitions has consequently been animated [2].

As a matter of fact, an important observation in nature is that the complex systems of interest are often open, and out of a thermodynamic equilibrium state. Their simplest condition is that of a nonequilibrium steady state. That is, a constant flux of some quantity (matter, energy,...) is typically involved and the state is, in general, not determined solely by external constraints, but depends upon their *history* as well. Un-

* Corresponding author.
*E-mail address:* jmarro@ugr.es (J. Marro).


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der such a nonequilibrium condition, as the control parameters—temperature or potential gradients, or reactant feed rates, for instance—are varied, the steady state may become unstable and be replaced by another (or, perhaps, by a periodic or chaotic state). Nonequilibrium instabilities are attended by ordering phenomena so analogous to those of equilibrium statistical mechanics that one may speak of *nonequilibrium phase transitions.* These are ubiquitous in physics and biology, and have also been described in the social sciences [2–5].

The simplest examples of nonequilibrium phase transitions occur in lattice models. The analysis of more realistic situations is presently confronted, among other problems, with the lack of a general formalism, analogous to equilibrium statistical mechanics. That is, nonequilibrium dynamics is not derivable from an energy function. One must actually find time-independent solutions of master or kinetic equations, which is a formidable task in practice. Therefore, general theoretical approaches are scarce. It is true that, for cases in which fluctuations are of minor significance, a macroscopic description, i.e. a set of partial differential equations is often preferable to a lattice model, for instance, in predicting a nonequilibrium phase diagram. However, such macroscopic descriptions imply mean-field behavior, while lattice models exhibit a range of critical phenomena and other details which are at least as interesting as in equilibrium [2]. The lack of theory also explains that most interesting information has been gained by means of computer simulations of the lattice models.

## 2. Neural cellular automata that efficiently recognize a pattern

As a first example of a complex lattice system that exhibits nonequilibrium phase transitions, let us consider an artificial neural network that was introduced and studied before [6]. This consists of a set of $N$ binary *neurons,* $\mathbf{s} = \{s_{\mathbf{x}} = \pm 1;\ \mathbf{x} = 1, \ldots, N\}$, evolving in time by stochastic equations,

$$\begin{aligned}\partial_t P_t(\mathbf{s}, \mathbf{J}) &= p\sum_{\mathbf{x}}\big[-\varpi_{\mathbf{J}}(s_{\mathbf{x}} \to -s_{\mathbf{x}})P_t(\mathbf{s}, \mathbf{J}) \\ &\qquad + \varpi_{\mathbf{J}}(s_{\mathbf{x}} \to -s_{\mathbf{x}})P_t(\mathbf{s}^{\mathbf{x}}, \mathbf{J})\big] \\ &\quad + (1-p)\sum_{\mathbf{x},\mathbf{y}}\sum_{J'_{xy}}\big[-\varpi(J_{xy} \to J'_{xy})P_t(\mathbf{s}, \mathbf{J}) \\ &\qquad + \varpi(J'_{xy} \to J_{xy})P_t(\mathbf{s}, \mathbf{J}^{xy})\big]. \end{aligned} \tag{1}$$

Here $\mathbf{J} = \{J_{xy} \in \Re;\ \mathbf{x}, \mathbf{y} = 1, \ldots, N\}$ is the configuration of synaptic intensities, and $\mathbf{s}^{\mathbf{x}}$ ($\mathbf{J}^{xy}$) stands for $\mathbf{s}$ ($\mathbf{J}$) after the change $s_{\mathbf{x}} \to -s_{\mathbf{x}}$ ($J_{xy} \to J'_{xy}$). The function $\varpi(J_{xy} \to J'_{xy})$ is taken independent of the current $\mathbf{s}$, and $\varpi_{\mathbf{J}}(s_{\mathbf{x}} \to -s_{\mathbf{x}}) = \varphi(2T^{-1}s_{\mathbf{x}}h_{\mathbf{x}})$, where

$$h_{\mathbf{x}} = h_{\mathbf{x}}(\mathbf{s}, \mathbf{J}) = \sum_{\mathbf{y}} J_{xy}s_{\mathbf{y}} \tag{2}$$

is a local field.

For $p = 1$, (1) reduces to the familiar Hopfield model in which the neurons evolve in the presence of a set of (frozen) synaptic intensities. It is assumed that these in some way contain information from a set of $P$ stored patterns, $\xi = \{\xi_{\mathbf{x}} = \pm 1;\ \mathbf{x} = 1, \ldots, N\}$, e.g., the Hebb choice $J_{xy} \propto \sum_{\mu=1}^{P} \xi_{\mathbf{x}}^{\mu}\xi_{\mathbf{y}}^{\mu}$ after appropriate normalization. Under such conditions, the model asymptotically tends to the equilibrium state for temperature $T$ and energy function, $H = \sum_{\mathbf{x}} h_{\mathbf{x}}s_{\mathbf{x}}$. This state sometimes corresponds to a configuration closely resembling one of the stored patterns; the system is therefore said to exhibit *associative memory*. However, this simple case is not sufficiently efficient for applications; e.g., errors when recovering a given pattern are large for most values of $N$, $P$ and $T$, and the steady state may not be "pure" but correspond to a mixture of two or more stored patterns.

For $p \to 0$, Eq. (1) transforms [2] into

$$\partial_t P_t(\mathbf{s}) = \sum_{\mathbf{x}}\big[\varpi(\mathbf{s}^{\mathbf{x}}; \mathbf{x})P_t(\mathbf{s}^{\mathbf{x}}) - \varpi(\mathbf{s}; \mathbf{x})P_t(\mathbf{s})\big], \tag{3}$$

where the transition probability per unit time is the superposition

$$\varpi(\mathbf{s}; \mathbf{x}) = \int \mathrm{d}\mathbf{J}\, f(\mathbf{J})\varphi\big[2T^{-1}s_{\mathbf{x}}h_{\mathbf{x}}(\mathbf{s}, \mathbf{J})\big]. \tag{4}$$

For appropriate choices of this superposition, i.e. of functions $f$ and $\varphi$, this system behaves qualitatively differents from the Hopfield case. That is, it can be shown—analytically in some cases and, more generally, by computer simulations—that a second-order (equilibrium) phase transition for $p = 1$ transforms for $p \to 0$ into a first-order (nonequilibrium) phase transition. This has some dramatic consequences concern-

ing the recognition of a given pattern out of a deteriorated image of it. In particular, for a wide and practically interesting range of $N$, $P$ and $T$, mixture states do not occur and the recovery process happens to be rather robust and accurate [6].

This study induced us to investigate a cellular automaton version of the original model. Firstly, the function $\varphi$ is properly determined; this choice importantly affects in practice some of the system properties, e.g., the nature of its phase transitions. The simulation then proceeds by choosing at random any of the stored patterns, say $\mu$, and updating all the neurons in the lattice assuming the set $J_{xy} = \xi^{\mu}_{\mathbf{x}}\xi^{\mu}_{\mathbf{y}}$, i.e. the synaptic intensities corresponding to the selected pattern. Next, this step is repeated again and again. The draw is performed in such a way that the time average for each local $J_{xy}$ gives Hebb's rule, $\langle J_{xy}\rangle \propto \sum_{\mu=1}^{P} \xi^{\mu}_{\mathbf{x}}\xi^{\mu}_{\mathbf{y}}$ (or, alternatively, any other learning rule one may use in the system definition).

The preliminary results that are available at the time of this writing reveal that this case exhibits a very robust and efficient process of pattern recognition. For most parameter values, starting from a perturbed pattern, the system rapidly transforms that configuration into the stored pattern that is closest to it. Fig. 1 shows the time evolution of the overlap between the actual state of the system and one of the stored patterns at

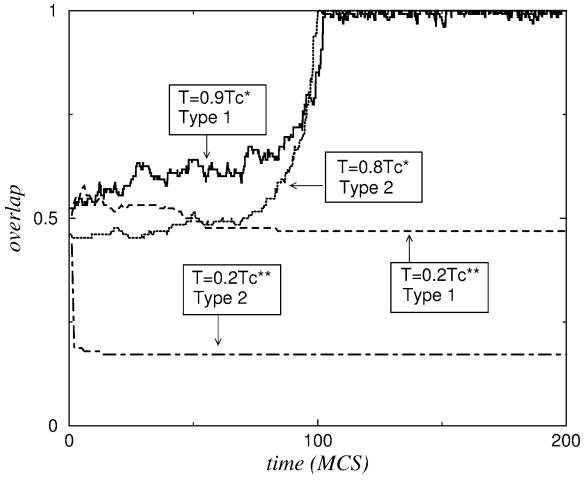


Fig. 1. The time evolution of the overlap in our cellular automata (two upper curves) is compared here with the Hopfield case (two lower curves). Note that, on the time scale of the experiment, only our system depicts a clear tendency towards saturation. See the text for more explanations.

indicated temperature. This is in units of the respective model critical temperature, either $T_C^* = 0.1$ and $T_C^{**} = 1$ for our system and for the Hopfield case, respectively. *Type* 1 here refers to the case in which the system stores $P = 150$ patterns whose sites are generated completely at random, so that each site is independent of the others; *type* 2 is for $P = 90$ stored patterns generated using the logistic map in the chaotic region of its parameter space, so that some correlation exits between sites. In both cases, our algorithm rapidly detects the pattern which is closest to the initial state. This behavior holds essentially for other values of the parameters.

The reason behind the *good* properties of our system seems to be that, for appropriate dynamics, the actual state only evolves noticeably at steps in which synapses correspond to the selected pattern [7]. This behavior opens the model to a wide range of possible applications.

## 3. Spinodal decomposition and criticality in driven fluids

The driven lattice gas (DLG) is a $d$-dimensional ($d = 2$ in the following) lattice gas at temperature $T$ in which transitions in (against) one of the principal lattice directions—say $\|$, to be referred to as the *field direction*—are favored (unfavored). For periodic boundary conditions, this induces a net current of particles along the field direction. At high $T$, the system is in a disordered state while, for half-filled lattices (the only case of interest in this paper), there is a second-order (nonequilibrium) critical point, below which the DLG segregates showing anisotropic, stripe-like configurations parallel to the field [2].

Establishing the universality class of the DLG is a main issue not only concerning a better understanding of these model properties but also much more generally, in relation to the theory of nonequilibrium phase transitions and critical phenomena. In fact, the DLG is recognized as one of the more intriguing model examples of nonequilibrium phenomena.

Recent field theory [8,9] motivated performing new and extensive computer simulations. These focused on the case of an "infinite" drive (particles along the field direction are not allowed to go backwards)

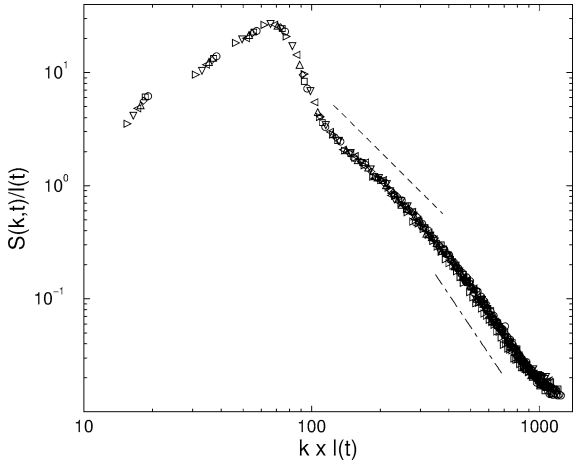


Fig. 2. Scaling of $S(k,t)$ for different times between $10^5$ MCS and $10^6$ MCS in a $128 \times 128$ system at low temperature, $T = 0.57T_C$. Two lines of slope $-2$ and $-3$, are indicated.

for both *large* squares and rectangular $L_\parallel \times L_\perp$ lattices of different, appropriate sizes. It has thus been demonstrated numerically that the DLG belongs to the same universality class as a lattice gas under a randomly fluctuating field [2] so that (using the renormalization group jargon) the particle current—which does not occur in the latter—is not a *relevant* feature of the DLG. Main critical exponents follow for both cases as $\beta = 0.33(1)$, $\nu_\parallel \simeq 1.25$ and $\nu_\parallel \simeq 2\nu_\perp$. These important results (that have more recently been confirmed independently [10]) can be interpreted within the context of the existing field theory [8,9]. It should be noted however, that the present form of this theory does not fit well the results of further numerical investigation of the same model. That is, studying small values of the field suggests that the DLG has no relation to the equilibrium lattice gas—so that one cannot go perturbatively from the latter to the case of small fields. There is some indication that the DLG belongs to the same universality class with $\beta < 1/2$ for any value of the field as long as the configurations are stripped [11]. If this is confirmed, the chances are that the DLG will again attract considerable attention during the coming years.

In fact, in addition to the above issue on criticality, there are further interesting questions concerning this model. One is the nature of its kinetic behavior as a configuration evolves from a disordered state to the stripped one. Extending the arguments first checked

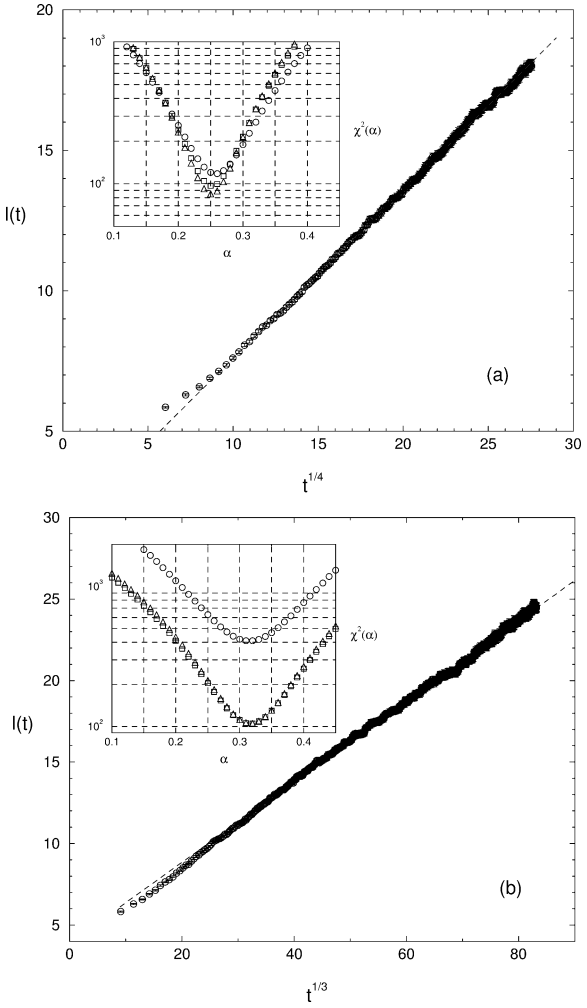


Fig. 3. In this figure we show $\ell(t)$ versus $t^\alpha$ for both $L_\perp \times L_\parallel = 64 \times 64$ (a) and $256 \times 64$ (b), and where $\alpha = 1/4$ and $1/3$ has been used, respectively. Notice that both plots follow a lineal law of the form $\ell(t) = at^\alpha + b$. $1/4$-behavior dominates the full evolution of the smaller system, while the larger one reaches the long time limit, thus showing $1/3$-behavior. In the insets we show $\chi^2(\alpha)$ for three different measures of the mean stripe width $\ell(t)$. Its minimum signals the experimental value of the growth exponent $\alpha$.

for systems that evolve towards equilibrium [12] one should perhaps expect *self-similarity* with time of the structure function. That is, as the system undergoes nucleation and then cluster coagulation according to a sort of spinodal decomposition, even though this is strongly anisotropic and will eventually lead to a nonequilibrium steady state, it seems reasonable to assume the existence of a unique relevant length. One

should expect this to be the length that characterizes the (transverse) clustering process in the system, say $\ell(t)$. Consequently, quantities changing with time should not depend explicitly on the time variable but only through $\ell(t)$. For example, the structure function $S(k,t)$ is expected to depict a scaled form $\tilde{s}(k')$, independent of $t$, when plotted accordingly,

$$S(k,t) \propto \ell(t)\tilde{s}\big(k\ell(t)\big). \tag{5}$$

This has recently been confirmed using the width of the stripes as the relevant length, as shown in Fig. 2. Moreover, we found that $\tilde{s}(k) \sim k^{-2}$ for large values of $k$, which is the generalization of Porod's law to DLG. This power law behavior, as compared to the $k^{-3}$ tail observed in bidimensional equilibrium binary mixtures, reflects the fact that coarsening in DLG is effectively a unidimensional process which takes place in the direction perpendicular to the field.

It has also been shown that $\ell(t) \sim t^{1/3}$, in general, as in standard spinodal decomposition [13] though the mechanisms leading to this behavior seem to be different. More specifically, we found that $\ell(t) = a(t/L_\parallel)^{1/3} + b$ for long enough times, where $a$ and $b$ are constants which depend on temperature, while for intermediate times we observe $\ell(t) \sim (t/L_\parallel)^{1/4}$ (see Fig. 3).

The analysis of all the above results on the dynamics of DLG allows us to conclude that the particle current does not play any important role in the late stage coarsening of DLG, the anisotropy being the relevant ingredient present in this process.

These facts motivate investigating experimentally spinodal decomposition in samples under nonequilibrium anisotropic conditions, e.g., scattering studies of fluids under shear.

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