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Growth of Ordered Domains Beyond a Dynamic Instability in Dissipative Systems

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We furnish evidence supporting our conjecture that the growth of structure which results at the onset of a center manifold in driven systems operating far from equilibrium can be described by a power law with a single exponent. More specifically, if the dissipative structure is contained in a center manifold and thus its stability is warranted, the linear dimensions for domains of organized spatial cells increase as $t^{1/2}$.

1. INTRODUCTION

The emergence of ordered structures in nonequilibrium driven systems is a field currently active investigation (Prigogine, 1984; Fernández, 1988*a*). A most challenging problem in this realm is to obtain *general* conditions which would warrant the permanence and stability of dissipative organizations (Fernández, 1988*b*). It has been established that, in a neighborhood of a critical dynamical regime, suitable constraints are furnished by the restriction that the dissipative structure must be contained within a locally-invariant and locally-attractive portion of phase space known as the center manifold (CM) (Fernández, 1988*a*,*b*). This hypersurface is normally calculated making use of what essentially is a mean field approach, with a free energy functional including third-order terms and terms representing the coupling between order parameters and fast-relaxing degrees of freedom (Fernández, 1988*b*). The CM coordinates are thus given by the order parameters which characterize the regime beyond the critical instability.

Perhaps the most elusive property of dissipative organizations, beyond the purely phenomenological realm, is the *cooperativity* among spatially-coupled cells which is responsible for the characteristic long-range order.

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Such cells, of course, are virtual entities (just like a Gibbs ensemble is a virtual object in equilibrium regimes), required to understand the onset of collective modes. However, models which make use of a cell decomposition, based on cooperative or synergistic interactions between subsystems, have proved successful in explaining the nature of intrinsic collective fluctuational modes in such different contexts as the onset of convective patterns (Fernández, 1988*b*) and the emergence of oscillatory and spatial patterns in open biochemical reactors (Prigogine, 1984).

The models for cooperativity have been tested against experimental evidence (Fernández, 1988*b*). The observable most widely used because of its experimental accessibility is the induction period for decay of metastable states (Langer, 1969): A homogeneous steady state is "quenched" within the critical regime and the decay of such a state occurs as a consequence of the propagation and amplification of nonequilibrium fluctuations along the CM. The terminal state is reached once all subsystems or cells belong to the CM and the quenched state is therefore regarded as metastable. The reader can easily trace an analogy with *spinodal decompositions*, familiar from condensed matter physics (Binder and Heermann, 1985). The similarity becomes all the more apparent once we have noticed that, in the case of nonequilibrium organizations, a critical "nucleus" is made up of a single cell contained in the CM.

The aim of this work is to study the growth of ordered domains during the amplification of long-wavelength fluctuations which occurs as time proceeds after the quench. This growth will be characterized by the time dependence of the linear dimension of ordered domains. Such domains, in turn, are comprised of cells which lie in the CM. At this point, we can anticipate the main result of this work: Computer simulation experiments provide evidence in support of the view that the growth of ordered domains is governed by a simple power law which makes our processes lie in the same universality class as previously-studied ordered-disorder phenomena (Binder and Heermann, 1985).

2. THE GROWTH OF ORDERED DOMAINS AT THE ONSET OF A CM

The existence of a CM entails a scaling of the intensity for the intrinsic random source and of the kinetic and control parameters of the system (Fernández, 1988*a*,*b*). The small characteristic parameter associated with the scaling is w/v, where v is the thermodynamic volume of the system and w is the volume of a virtual spatial cell. Thus, the existence of a CM allows for the construction of a nonequilibrium ensemble of coupled subsystems whose dimensions are determined by the scaling. The parameter $\langle y \rangle$ which

we plan to investigate is defined as follows:

$$\langle y\rangle = \langle (v_{\text{org}}/w)^{2/3}\rangle \tag{1}$$

where the angular brackets denote thermal or statistical average over the ensemble of subsystems and v_{org} is the volume, measured in w units, of the reunion of organized subsystems adjacent to a given organized subsystem. Thus, if $\mathscr{B}$ denotes a generic subsystem, we get

$$(v_{\text{org}}/w)(\mathscr{B}) = \begin{cases} 0 & \text{if } \mathscr{B} \text{ is not organized} \\ 1 & \text{if } \mathscr{B} \text{ is organized, but isolated} \\ n & \text{if } \mathscr{B} \text{ is surrounded by } n-1 \text{ organized cells} \end{cases} \tag{2}$$

The exponent 2/3 in equation (1) was chosen so that we can establish the time-dependent behavior of the linear dimensions of ordered domains. The choice is justified since we shall furnish evidence in support of the power law

$$L(t) \approx t^{1/2} \tag{3}$$

where L represents the linear dimension.

The average indicated in equation (1) is given by

$$\langle y\rangle = (w/v) \sum_{\mathscr{B}} [v_{\text{org}}(\mathscr{B})/w]^{2/3} \tag{4}$$

In order to establish the time-dependent behavior of this function, it is essential that we make use of the model recently implemented (Fernández, 1988*a*) for the propagation and amplification of fluctuations along the CM. For the sake of clarity, we outline here the basic tenets of the model.

1. Every (virtual) subsystem has volume w and the partition of the thermodynamic volume v is made according to the CM decomposition. All subsystems are assigned an identical coarse-grained phase space, denoted by Σ. The coarse graining is determined by the space of realizations of the random source which results after a CM reduction has been performed on the original master equation. This starting equation involves all the degrees of freedom in the system. By a CM reduction we mean a scaling operation which yields, to leading order in w/v, a "smeared" Fokker–Planck equation for the order parameters or CM coordinates. The phase space Σ can be specified by equivalence relations, where two microstates which are equivalent are regarded as one and the same. The microstates are equivalent if and only if: (a) they have associated the same macrostate (as defined by a particular value of the CM coordinates) and (b) there exists a phase trajectory joining them which does not entail any variation in the random source term of the smeared Fokker–Planck equation.

2. The time evolution of the system in a metastable state is described by a probability distribution p, given by

$$p = \{p(A)\}_{\text{all } c(A) \text{ in } \Sigma}; \qquad p(A) = \langle \chi(A) \rangle \tag{5}$$

Here A denotes an arbitrary microstate in a cell, $c(A)$ denotes the class of all equivalent microstates, and $\chi(A)$ is the characteristic function of $c(A)$, defined over Σ. Thus, $p(A)$ gives the probability that a cell is in a microstate equivalent to A.

3. In order to study the growth of ordered domains of cells, we must restrict ourselves to a subspace of Σ. This subspace, denoted Δ, contains all classes of microstates whose macrostates belong to the CM, excluding the attractor. This restriction is properly justified in Fernández (1988*a*) and must be introduced since the lifetime of an organized cell in the attractor is infinite, whereas the lifetime of a cell in the CM excluding the attractor is finite (this portion is strictly *locally* attractive). Thus, the evolution of organized cells, which behave as information carriers, is given by the distribution

$$P = \{p(B)\}_{\text{all } c(B) \text{ in } \Delta} \tag{6}$$

The time evolution of P depends on the cell correlations

$$S_{AB} = \langle\langle \chi(A, \alpha) \chi(B, \beta) \rangle_\alpha \rangle_\beta \tag{7}$$

where α and β label replicas. The evolution of information carriers is governed by the system of equations [there is one equation for each cell $c(B)$ in Δ]

$$\langle \partial \chi(B)/\partial t \rangle = \left[\sum_{c(A) \text{ in } \Delta} (\partial S_{AB}/\partial t)(1-x) \langle \chi(A) \rangle \right] - N^{-1} \langle \|f\|^2 \rangle^{1/2} \langle \chi(B) \rangle \tag{8}$$

where x is the order parameter that gives the probability that a subsystem lies in the CM, excluding the attractor:

$$x = \sum_{c(B) \text{ in } \Delta} p(B) \tag{9}$$

Thus, $1-x$ gives the probability that a particular subsystem is disorganized or lies in the attractor. This implies that a term proportional to $1-x$ which depends on A and B gives the probability per unit time that a subsystem in cell $c(A)$ induces a subsystem whose microstate is outside Δ to become organized by evolving to $c(B)$ (which, obviously, must belong to Δ). The remaining term in the rhs of equation (8) reflects the fact that the CM acts as a *transient* source of free energy, since each information carrier has a finite lifetime given by the reciprocal of the effective diffusion

coefficient. This coefficient is specified by the strength of the random source $f=f(t)$ in the smeared Fokker-Planck equation and by the dimension N of the CM.

At this point we are in a position to investigate the time behavior of ordered domains. For the purpose of adequate verification of equation (3), we introduce the variable Y, which scales with the previously-defined dimensionless variable y as follows:

$$Y = yM \qquad (M \text{ in seconds}) \tag{10}$$

Given the definition of y given by equation (1), the conjecture presented in equation (3) could be confirmed if Y is shown to be linearly dependent on time.

A simulation making use of working equations (4) and (8) has been carried out with the following choice of parameters: $v/w = 10^3$; $\|f^2\|^{1/2} = 10^{-6}\,\mathrm{s}^{-1}$; $\dim(\Sigma) = 3 \times 10^3$; $N = 2$ and $\partial S_{AB}/\partial t = 10^{-6}\,\mathrm{s}^{-1}$ for all A and B

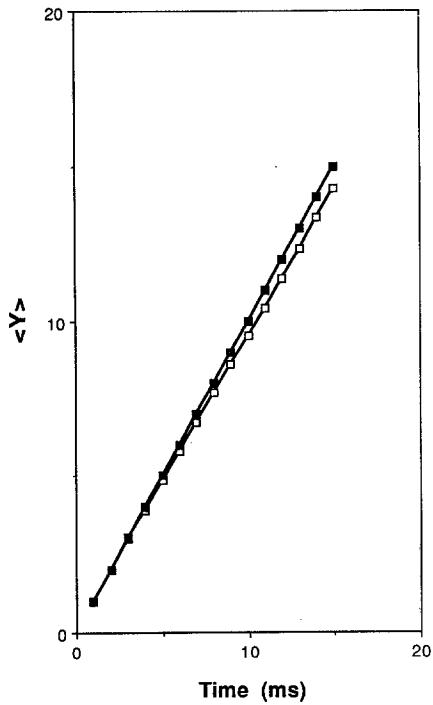

Fig. 1. Growth of ordered domains beyond a dynamical instability at the onset of a center manifold. The solid squares correspond to a hypothetical purely linear time dependence, whereas the plot with open squares represents the result of our simulation. Parameters are as indicated in the text.

in Δ. The free parameter has been fixed at $M = 10^{-3}$ s. The plot with open squares presented in Figure 1 was obtained by means of the simulation and the plot with solid squares reflects a hypothetical purely linear behavior. The simulation conclusively supports the power law conjectured in equation (3). Nevertheless, however suggestive or compelling that evidence might be, producing an analytical proof remains a challenging open problem.

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