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Towards a global classification of excitable reaction–diffusion systems

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Abstract

Patterns in reaction–diffusion systems near primary bifurcations can be studied locally and classified by means of amplitude equations. This is not possible for excitable reaction–diffusion systems. In this paper we propose a global classification of two variable excitable reaction–diffusion systems. In particular, we claim that the topology of the underlying two-dimensional homogeneous dynamics organizes the system's behavior. We believe that this classification provides a useful tool for the modeling of any real system whose microscopic details are unknown. © 2000 Published by Elsevier Science B.V. All rights reserved.

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Many dissimilar experimental and model reaction–diffusion systems display similar behavior. This raises the question of whether a classification can be found so that seemingly unrelated systems with similar dynamics can be understood as belonging to the same equivalence class. We argue in this paper that a global classification is possible for reaction–diffusion systems whenever the underlying homogeneous dynamics can be mapped onto a *planar flow* (i.e., a flow in R^2). This classification is done in terms of *model families* [2] that are largely determined by the homogeneous dynamics. In support of our conjecture we analyze experiments done in an open reactor using the FIS (Ferrocyanide-Iodate-Sulfite) reaction [2–4] and two reaction–diffusion models [5,6] that display similar patterns to those of the experiment, even though they are not accurate models of the FIS kinetics. We explain these common behaviors by noting that they all have similar homogeneous dynamics and discuss the main features of their model family.

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[2] The idea of obtaining qualitative universality classes in terms of model families is already present in [1].

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The classification of system behaviors lies at the heart of dynamical systems theory and here the normal form theorem is one of the main achievements [7]. It states that close to a bifurcation point the dynamics of any sufficiently smooth system can be reduced to a simplified set of equations that is locally topologically equivalent to the full vector field [3]. The normal form approach is local in both phase and parameter space. Thus, classifications based on it provide generic descriptions only when the system is near threshold. For this reason, the patterns that occur in the *excitable systems* that we discuss in this paper cannot be classified with normal form techniques.

Excitability is a common dynamical behavior that occurs, for example, in the kinetics of neuronal membrane potentials [9], in semiconductor lasers with feedback [10] and in a variety of chemical reactions [2]. The picture of excitability we use is defined in terms of the spatially uniform dynamics. It assumes the existence of a stable fixed point (a spatially uniform stationary solution) such that perturbations above a threshold result in a large excursion in phase space before the systems decays back to the fixed point. A spatially uniform excitable dynamics can result in wave propagation or in multistability when spatial variations are allowed. In particular this is true when the coupling is diffusive, i.e., for *reaction–diffusion* systems (see e.g. [5]). Since these behaviors arise from a finite perturbation of the spatially uniform steady state, classifications based on local normal forms cannot be used.

We now consider a reaction–diffusion system whose homogeneous dynamics can be mapped onto a planar flow. Because of the limited set of asymptotic behaviors allowed by flows in R^2 [4] they are particularly easy to classify. Given the fixed points of the flows there is a finite set of possible asymptotic behaviors and transitions among them [5]. Thus, we can classify *families* of planar flows that smoothly deform into one another by varying parameters [12]. It is important to note that this is a *global* description, as opposed to the local one provided by near threshold normal forms. This global description is valid for the spatially uniform dynamics. When diffusion terms are added the planar system becomes high-dimensional. We conjecture that there exists a natural global description for the high-dimensional reaction–diffusion system that is the direct analogue of the known global description of the two-dimensional planar system. This means there should exist a *model family* of two coupled reaction–diffusion equations which displays the same patterns and transitions among them as any other member of the class. Our conjecture is that, for reaction–diffusion systems which in the homogeneous limit can be described by planar flows, these model families are mainly determined by the homogeneous dynamics.

Given a set of two reaction–diffusion equations with bounded diffusion terms, the local dynamics at each time and point in space is given by a planar flow which corresponds to a (not necessarily small) perturbation of the original homogeneous flow [6]. Thus, *the model family of the class which a particular system belongs to should not only display homogeneous behaviors that are topologically equivalent to those of the system we are trying to classify, but it should also contain its closest perturbations.* Since flows in R^2 with a finite number of fixed points have a finite set of asymptotic behaviors and can undergo a countable set of bifurcations, we then expect to find a countable set of model families. This gives the desired classification of excitable systems describable by pairs of reaction–diffusion equations.

[3] Normal form analysis provides a powerful tool for modeling real systems because it is independent of the specific details. If the type of bifurcation is known then it follows that there is a set of variables in which the evolution is given by dynamical equations of a known form. It is sometimes possible to infer from experimental data which physical quantities these variables may correspond to and thus to obtain a dynamical model. See e.g. [8].

[4] They are restricted by the Poincaré–Bendixon theorem, see e.g. Ref. [11].

[5] We also need to know how the flow behaves near infinity, which can usually be regarded as a collection of fixed points.

[6] We must point out that we do not mean small perturbations. Indeed, the nice feature of planar vector fields that we exploit in this paper is the fact that we can have (generic) global bifurcation sets for their families (by restricting the number of fixed points). This implies that we may know a-priori all the topological changes that a given flow may suffer, no matter how big a perturbation is needed in order to generate such change.

Let us give a qualitative argument of why the global classification of flows in R^2, which only holds in the spatially homogeneous limit, may carry over to the (infinite-dimensional) spatially extended case, independently of how 'big' the diffusive terms may be. Let us consider a set of reaction-diffusion equations of the form $\partial_t u = D_u \nabla^2 u + f(u,v)$, $\partial_t v = D_v \nabla^2 v + g(u,v)$. For the sake of the argument, let us assume that the terms $D_u \nabla^2 u$ and $D_v \nabla^2 v$ are time-independent and that they vary continuously with the spatial point, $\boldsymbol{x}$ [7]. Then, the reaction-diffusion system can be viewed as a collection of planar flows, with $\boldsymbol{x}$ playing the role of a parameter. The flows change when we move from one spatial point to the next one, but, due to Peixoto's theorem [7], there are open sets of $\boldsymbol{x}$ for which all the flows are structurally stable and topologically equivalent to one another. These regions are separated by 'boundaries' on which the flows are not structurally stable. What flows are in this collection? We may assume that in one of these open sets the flows are topologically equivalent to that of the spatially homogeneous system, $\dot{u} = f(u,v)$, $\dot{v} = g(u,v)$. This happens in the examples discussed later in this paper. Then, a collection of topologically distinct flows can be easily constructed by exhaustion (in the very same way in which a global bifurcation set for planar flows with at most a certain number of fixed points and periodic orbits can be constructed [12]). Furthermore, if we limit the number of fixed points and periodic orbits of the flows, there is a finite set of topologically distinct flows. Now, even if this set is finite, in principle we could have as many disconnected open sets in $\boldsymbol{x}$ as we wished, each with structurally stable flows. However, with some regularity conditions on the way in which the diffusive terms behave, it should be possible to restrict this number of disconnected spatial regions. So far, we have assumed that the terms $D_u \nabla^2 u$ and $D_v \nabla^2 v$ are time-independent. In the time-dependent case, we could think again of a collection of planar flows. In this case the boundaries between the regions will move, some regions will disappear momentarily and reappear at some other time. We do not have a clear understanding of under which conditions, in this case, different systems could be 'dissected' into disconnected open regions that behave similarly in time. However, as we show in the examples presented in this paper, the equivalence seems to hold also for (at least some) time-dependent solutions. We now develop the necessary tools to discuss this particular application.

[7] In principle, this will only happen if u and v are also time-independent. However, this will help understand our argument in the general case.

We first develop a simple geometric model of excitability in R^2 suitable for our purposes. We consider a set of equations $\dot{u} = f(u,v)$, $\dot{v} = g(u,v)$, with only one attractor: a stable fixed point, $\bar{x} \equiv (\bar{u},\bar{v})$. Excitability implies that the flow lines turn around before coming back to $\bar{x}$. The simplest situation with this property is depicted in Fig. 1(a), that corresponds to the case in which $\bar{x}$ (the square) is the only limit set of the flow. This flow can generically undergo a 'saddle-repellor', a saddle-node or a Hopf bifurcation, leading to the flows shown in Fig. 1(b)–(d), respectively. The fixed point $\bar{x}$ is stable in all cases but in (d), where there is an attracting limit cycle. In Fig. 1(b) and (c) it coexists with a saddle (the diamond) and a repellor (the white circle) or a node (the black circle). While the Hopf bifurcation requires that $\bar{x}$ be a spiral, which is unrelated to it being excitable, the saddle-node and saddle-repellor

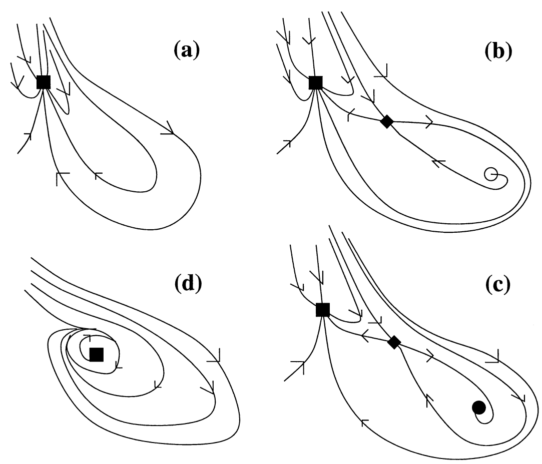

Fig. 1. Planar flow with one excitable fixed point (a) and its closest perturbations (b)–(d).

bifurcations may be linked to the excitability of $\bar{x}$. In fact, excitability is related to the existence of a separatrix, which becomes the stable manifold of the saddle after it is born. Also, the turn around of the flow lines implies that the orientation of the *null-clines* (the curves that satisfy $f(u,v)=0=g(u,v)$) is such that, by not too large a perturbation, they can eventually become tangent at a point. Generically, when this happens, a saddle-node or saddle-repellor bifurcation occurs. These two types of bifurcations 'meet' at a codimension two point, the Takens–Bogdanov point. The simplest family that contains the flows in Fig. 1(a)–(c) outside a neighborhood of $\bar{x}$ is given by the Takens–Bogdanov normal form [8]: $\dot{u}=v,\ \dot{v}=\mu_1+\mu_2 v+u^2+uv$. It is easy to modify these equations so that they also describe the behavior at and near $\bar{x}$ (see e.g. [10]). Flows of this 'extended' family with only one fixed point have the inflection of the flow lines necessary for excitability. We may thus call it a general model of excitability in R^2, for systems with one fixed point. Since the family contains all the relevant perturbations of the flow in Fig. 1(a), it is also suitable in the extended case [9].

We now consider a reaction–diffusion system with an underlying planar homogeneous dynamics that has only one stable but excitable fixed point. As a model family of its class we choose a two-variable reaction–diffusion system that, in the homogeneous limit, contains the flows in Fig. 1(a)–(c). Now, any affine transformation $(u,v)\to\mathscr{M}(u-u_0,v-v_0)$, with $\mathscr{M}$ a constant 2×2 matrix, will give another family with an equivalent homogeneous dynamics and, in many cases, the right 'winding' of the flow lines. If we introduce such a transformation in a set of the form $\partial_t\tilde{u}=D_u\nabla^2\tilde{u}+\tilde{f}(\tilde{u},\tilde{v}),\ \partial_t\tilde{v}=D_v\nabla^2\tilde{v}+\tilde{g}(\tilde{u},\tilde{v})$, we get a new set with cross-diffusion terms. Thus, once we have any family, $\dot{u}=f(u,v),\ \dot{v}=g(u,v)$, with the 'right' homogeneous dynamics, we expect, in most cases, that each (stationary) pattern of the system of interest be equivalent to a pattern of a flow in the family

$$\partial_t u=D_{uu}\nabla^2 u+D_{uv}\nabla^2 v+f(u,v),$$
$$\partial_t v=D_{vu}\nabla^2 u+D_{vv}\nabla^2 v+g(u,v). \qquad (1)$$

Since it is possible to get rid of cross-diffusion by a simple transformation, it should always be possible to choose a *particular* model family without it.

Now we discuss three concrete examples of systems with the excitable homogeneous dynamics discussed above. Consider the FIS reaction, which produces the patterns of Fig. 2 [3,4]. In the well-mixed (i.e., spatially homogeneous) case, it is known to exhibit excitability, bistability and oscillations [13]. These homogeneous behaviors can be described by planar dynamical systems. The dynamical models of the system (a set of 10 ODE's) [14,15] show that for the parameter values used in all the experiments, there is a separation of time-scales that allows the reduction of the original 10-dimensional system to a planar one. This planar system can have at most three fixed points, one of them a saddle. Experimentally, only stable solutions can be observed. The existence of the unstable fixed points and other limit sets are deduced from the model.

In this paper we discuss the replicating spots (Fig. 2(a)) and lamellar structures (Fig. 2(b)) that are found when there is only one homogeneous stationary solution, the low pH fixed point, and it is stable [3,4]. Experimentally, the spots are initiated by finite perturbations of the low pH state. This reflects its excitability. Thus, a model family like the one sketched before should reproduce at least some of the observed patterns. The transition from spots to lamellae shown in Fig. 2 is observed as the concen-

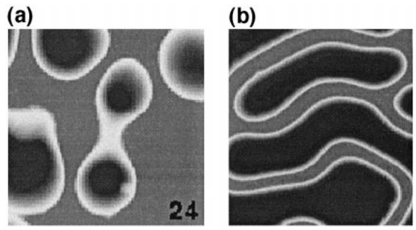

Fig. 2. Transition from replicating spots to labyrinthine patterns in the FIS reaction when the homogeneous system approaches the saddle-node saddle-repellor bifurcation.

[8] This normal form can either have a plus or a minus sign in front of the uv term (see [7]).

[9] In order to describe certain patterns it may suffice that the model families contain only a proper subset of all perturbations. For the example discussed here the flow of Fig. 1(d) is unnecessary.

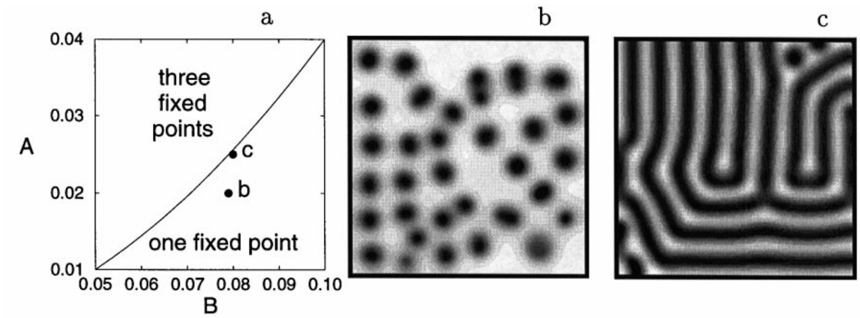

Fig. 3. A partial bifurcation set for the homogeneous Gray–Scott model (a) and two examples of patterns that occur for the parameters indicated in (a) when $D_u = 1$ and $D_v = 0.5$. The line corresponds to the curve of saddle-repellor bifurcations of the homogeneous system.

tration of ferrocyanide, $[Fe(CN)_6^{4-}]$, is decreased [3,4]. The homogeneous system approaches a saddle-node bifurcation as $[Fe(CN)_6^{4-}]$ is decreased. Below a critical value there are three fixed points (a low pH one, a high pH one, and an intermediate pH saddle). Above this value only the low pH fixed point persists. We will show that both the patterns and this transition are contained in the model family we propose.

The Gray–Scott and Fitzhugh–Nagumo models display spot replication and lamellar patterns. The Gray–Scott model is given by [5,16,17]:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + A(1-u),$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - Bv, \tag{2}$$

and it has been shown to behave similarly to the experiment [3,4]. The Fitzhgugh–Nagumo model [18,6], can be written as:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - \alpha(v + a_1 u - a_0),$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + v - v^3 + u. \tag{3}$$

The homogeneous dynamics of both models is a flow in R^2. Furthermore, the families described by Eqs. (2) and (3) contain the flows of Fig. 1(a)–(c). Thus, both systems have the 'right' homogeneous dynamics to construct model families of one another and of the FIS reaction. We conclude that all these systems belong to the same equivalence class. Furthermore, for the qualitative comparison we present, cross diffusion terms are not necessary and either Eq. (2) or (3) can be used as the model family for this class.

We show in Figs. 3 and 4 snapshots of some of the patterns obtained in numerical simulations of Eqs. (2) and (3), respectively, when the systems have only one stable but excitable fixed point. We observe spot replication and labyrinthine patterns. As in the experimental system, we observe a transition from spots to lamellar patterns as the homogeneous systems approach the saddle-node (saddle-repellor) bifurcation (see the partial bifurcation sets shown in Fig. 3(a) and Fig. 4(a)) [10]. We can provide a rough explanation for this if we think of stationary solu-

[10] We note that the patterns of Figs. 3 and 4 were obtained for $D_u/D_v > 1$, with u the inhibitor and v the activator in both cases. In fact, the analysis of [16,17] and [19] show that non-homogeneous solutions to the Gray-Scott model exist in the limit of a slowly diffusing activator. The same condition is satisfied in the simulations of [6]. The more detailed analysis we will present elsewhere [12] indicates that this is a necessary condition for all systems in the parameter regime considered in this paper. In the 2 variable model of the experimental system, H^+ is the activator and HSO_3^- is the inhibitor. As pointed out in [3,4], a slowly diffusing activator does not seem reasonable, since protons (H^+) diffuse rapidly compared to the other species. However, the reduction from 10 to 2 variables in the FIS model kinetics involves replacing the chemical steps $2H^+ \to I_2$, $I_2 + HSO_3^- \to 3H^+$ by the single one $2H^+ + HSO_3^- \to 3H^+$. Thus, the activator of the 2 variable model has an effective diffusion coefficient that is determined by both the protons and iodine, I_2 [12]. This effective diffusion coefficient may be small, since iodine binds to the gel which, in turn, substantially reduces its own effective diffusion coefficient.

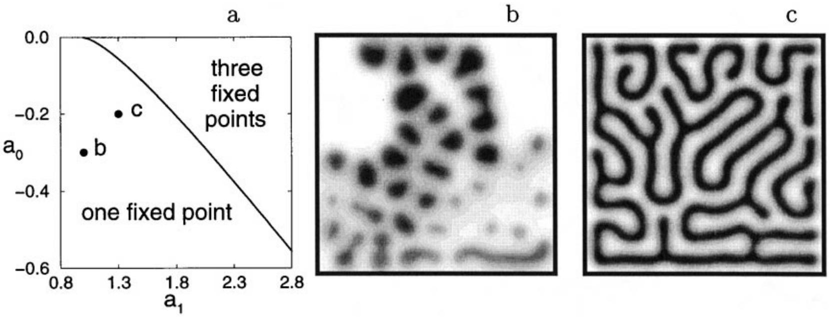

Fig. 4. Similar to Fig. 3, but for the Fitzhgugh–Nagumo model. The examples in (b) and (c) were obtained for $D_u = 1$ and $D_v = 0.166$.

tions and regard diffusion as a perturbation on the homogeneous dynamics at each spatial point. In this sense, diffusion makes the system cross the saddle-node (or saddle-repellor) bifurcation. It is clear that the closer the homogeneous system is to the bifurcation, the smaller must be the perturbation and thus $\nabla^2 u$ and $\nabla^2 v$. For this reason, more spatially extended patterns with smaller Laplacians (such as lamellae) can be supported when the homogeneous system is closer to the bifurcation point.

We have proposed a global classification scheme for excitable reaction–diffusion systems in terms of model families whose choice is based on their underlying homogeneous dynamics. The main purpose of such a classification is the modeling of real extended systems whose detailed underlying microscopic dynamics is unknown. Using this approach, we could explain some common behaviors observed in the FIS reaction and in Eqs. (2) and (3) as a consequence of their belonging to the same equivalence class (for the parameter values discussed in this paper). As far as we know, this is the first time that a connection between these apparently dissimilar systems has been established based on the topological features of their dynamics. In this example, the corresponding model family is organized around a Takens–Bogdanov point [11]. We call it the *Takens–Bogdanov model of excitability*. Families with other types of homogeneous dynamics will serve as templates for other classes of excitable systems. We believe that this classification approach will be possible whenever the homogeneous dynamics can be mapped onto a planar flow. The fact that limit sets of planar flows are so restricted may be the explanation of the ubiquitous presence of certain patterns in diverse systems. For example, this might be the reason that the complex Ginzburg–Landau equation reproduces behaviors outside its range of applicability as a near-threshold normal form. We also think that some transitions observed in spatially extended systems could be understood in terms of bifurcations of the local (homogeneous) dynamics because this local homogeneous dynamics was two-dimensional [21].

[11] The existence of a Takens–Bogdanov point has also been linked to spot replication by Y. Nishiura, D. Ueyama (to be published) and to Turing instabilities by Pearson and Horsthemke in Ref. [20].

Acknowledgements

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