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Turbulent states in a reaction-diffusion system with period-doubling bifurcations

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ABSTRACT

We investigate the spatially extended Hastings–Powell model in one and two dimensions with constant diffusion coefficients and nonflux boundary conditions. Nowave zones, spirals and chaos are found. An absolute instability of the spirals produces a transition to chaos. A constant number of defects, linearly increasing with the bifurcation parameter of the system is found, i.e. there do not exist defect-creation or defect-destruction events. Defects behave as hard disks, with translational degrees of freedom, which result from a cooperative interaction between pairs of defects.

1. Introduction

Nonlinear phenomena and spatiotemporal patterns such as spiral waves, meandering and chaos have been observed experimentally in various biological, chemical and physical systems. In chemical systems they have been observed in the Belousov–Zhabotinsky (BZ) reaction, the $CO + O_2$, $NO + CO$ and the $NO + NH_3$ reactions on Pt surfaces, etc. [1–7]. They have also been found in numerical simulations of reaction-diffusion systems and in the complex Ginzburg–Landau equation [7–10].

There has been much interest in understanding the generic rules governing nonequilibrium pattern dynamics, though the studies have been mostly limited to simple cases in which the concerned system is either excitable, bistable or simply periodic (i.e. period 1). In excitable or simply periodic systems, the fundamental property of a spiral wave is a topological (phase) singularity that constitutes the tip of the spiral [11]. Spiral waves can destabilize in many different ways. For instance, they may begin to meander or to drift, a scenario that has been attributed to a Hopf instability. Another common instability is the breakup of the spiral wave: either the core or the far field of the spiral breaks up into a turbulent region with complex spatiotemporal behavior [12].

Spiral waves can also exist in complex oscillatory media where the local dynamics exhibits period-doubling or even chaotic behavior. In such complex oscillatory regimes, the new feature that appears is the existence of a line defect across which the phase of the oscillation changes by 2π. In fact, the line defects are an essential property of complex periodic spiral waves, i.e. complex spiral waves cannot exist without line defects. The dynamic of the line defects has been investigated in systems where the spatially homogeneous system itself exhibits a period-doubling route to chaos, i.e. the Rössler model, which also constitutes a simplistic model of a chemical reaction [13–15]. Line defects have also been observed experimentally in the BZ reaction [16].

The period-doubling or Feigenbaum scenario is a route to chaos that has also been observed in the transition from regular oscillation to chaos in a number of chemical reactions such as $NO + CO/Pt\{100\}$ and $NO + H_2/Pt\{100\}$ [17,18]. However, in contrast to the attention received by the spiral dynamics, the spatiotemporal chaotic states of systems undergoing period-doubling bifurcation have not been fully investigated yet [14,15].

In the present work, we investigate the spatially extended Hastings–Powell model with constant diffusion terms. Like the well-known Lotka–Volterra model, the Hastings–Powell (HP) model has also been originally introduced in the context of ecological nonlinear processes, though it more generally describes a complex autocatalytic reaction whose temporal evolution is described by a set of a three differential equations [19].

The HP model shows a period-doubling route to chaos and in the present work we characterize its spatiotemporal behavior in both one and two spatial dimensions. Spiral waves and defect-induced turbulent states are found in 2D. In particular, we found that turbulent states have quite different characteristics compared with similar states in excitable systems. In excitable systems, turbulent states are characterized by a dynamic process involving creation and destruction of defects. The number of defects fluctuates and the state is characterized by performing defect statistics [20,22,23]. In the present work, we found defect-induced turbulent states without neither creation nor destruction of defects, i.e. the number of defects is constant. Furthermore, the number of defects increases with the bifurcation parameter of the system.

The present work is organized as follows: in Section 2 we describe the model and details of our calculations. Section 3 summarizes our results, and Section 4 our conclusions.

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2. The model

Though the Hastings–Powell (HP) model has been originally developed to describe a three-species food chain (with X being the population of the species at the lowest level, Y the population of the species that preys upon X, and Z the population of the species that preys upon Y), it also constitutes a dynamic model to describe a nonlinear reaction system. The first and the second terms on the right hand of Eq. (1) (see below) represent an autocatalytic process and a second-order recombination step, respectively. In Eqs. (1) and (2) the function $f_1(x)$ given by Eq. (4) represents an effective rate constant of a process involving, under steady-state conditions, the formation of an intermediate species (with consumption of y) with two different reaction pathways, one of them involving the consumption of x and the production of y. Identical considerations hold for $f_2(y)$.

The nondimensionalized HP model can be written as

$$\frac{\partial x}{\partial t} = x - x^2 - f_1(x)y \tag{1}$$

$$\frac{\partial y}{\partial t} = f_1(x)y - f_2(y)z - d_1 y + D_y \nabla^2 y \tag{2}$$

$$\frac{\partial z}{\partial t} = f_2(y)z - d_2 z + D_z \nabla^2 z \tag{3}$$

where x, y and z are the dimensionless versions of X, Y and Z, respectively, and

$$f_i(u) = \frac{a_i u}{1 + b_i u} \tag{4}$$

Table 1 summarizes the parameter values used in the present work.

In Eqs. (2) and (3) the diffusional terms spatially extend the dynamic system. It is assumed that x diffuses very slowly in comparison to y and z. We also introduced constant diffusion coefficients for y and z, though the spatiotemporal behavior of an extended system depends on the dimension of the dynamic system, the existence of noise and the characteristics of the transport processes [21–25].

Simulations were performed in one and two dimensions on grids of 400 and 256×256 points, respectively, with nonflux boundary conditions. We found our results to be independent of the lattice size in both one and two dimensions. In 2D we performed simulations on $L \times L$ lattices with $L = 128$, $L = 256$ and $L = 512$, respectively, and the minimum value of $L = 256$ was chosen to obtain quantitative results independent of the lattice size for the whole range of b_1.

We used an explicit Euler integration scheme for both the reaction and the diffusion terms. For the latter, a five-point stencil with a mesh size $\Delta x = \Delta y = 1.0$ was used. Smaller mesh sizes have not been found to produce qualitatively different results. An integration time step $\Delta t = 0.01$ was used to ensure mathematical stability. Results were checked to be independent of the integration step for sufficiently small values of Δt.

Table 1
Parameter values used in the present work (see Eqs. (1)–(3))

Parameter	Value
a_1	5.0
b_1	2.3–3.5
a_2	0.1
b_2	2.0
d_1	0.45
d_2	0.01
D_1	0.2
D_2	0.2

3. Results

The dynamic behavior of the HP model has been numerically explored in Ref. [19] as the parameter b_1 varies. The bifurcation diagram showed a period-doubling route to chaos, and Fig. 1 shows it in the range of b_1 values explored in the present work (i.e. $2.3 \leqslant b_1 \leqslant 3.5$). The diagram in Fig. 1 was constructed by varying b_1 in steps of 0.01, computing successive maxima of z.

The first bifurcation occurs at $b_1 = 2.41$, while at $b_1 = 2.62$ a four-period fix point appears first. The first bifurcation to an eight-period fix point occurs at $b_1 = 2.98$. In Ref. [19] it has been argued that the dynamical behavior could depend on the initial conditions. We also found this dependence in our spatially extended model and for this reason we always initiated our simulations from a given initial condition, i.e. a fully developed spiral as is obtained at $b_1 = 2.907$ (see below).

Fig. 2a shows the phase diagrams of the dynamic system for some characteristic values of b_1, and Fig. 2b shows the corresponding spatiotemporal diagrams of the 1D spatially extended system with $D_y = D_z = 0.2$ and nonflux boundary conditions. The initial perturbation consists of a linear gradient of y, and we found our results to be independent of the lattice size. At $b_1 = 2.95$ the attractor starts to exhibit the well-known upside down teacup form, which is fully developed at $b_1 = 3.1$. The 1D spatially extended system shows backfiring as a transient to a disordered state. In the backfiring a traveling pulse splits and creates a new pulse traveling in the opposite direction. Two pulses traveling in opposite directions can collide and annihilate themselves. These creation and destruction processes yield to a disordered state and disappear at very long time. At $b_1 = 3.46$ a nowave region appears again.

Below we use the results summarized in Figs. 1 and 2 to interpret our two dimensional simulations. Fig. 3 shows a phase diagram of the 2D spatially extended system (in a lattice $L \times L$, with $L = 256$) in the range $2.3 \leqslant b_1 \leqslant 3.5$. The phase diagram was constructed by varying b_1 in steps as small as 0.001. In the range $2.3 \leqslant b_1 < 2.86$ there is a nowave zone; only decaying amplitude oscillations are supported by the system. As we mentioned above, the spatiotemporal behavior of the system depends on the initial conditions, and for this reason we always start the simulation from the same initial condition corresponding to a well-developed spiral. Other more disordered states were also used, but in these cases spatiotemporal responses were not found. The above-mentioned dependence of the spatiotemporal behavior on the initial conditions remains even at larger lattices but, for a given initial

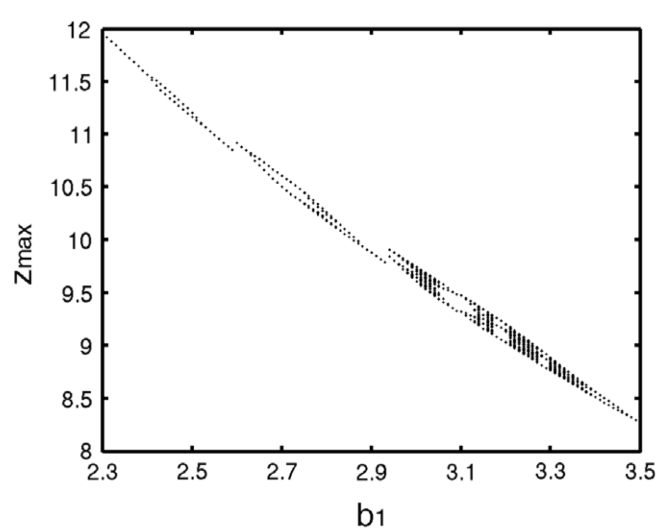

Fig. 1. Bifurcation diagram of the HP model showing the period-doubling route to chaos as b_1 varies.