PHYSICAL REVIEW E **70**, 035203(R) (2004)

Topological characterization of spatial-temporal chaos

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(Received 26 August 2003; published 27 September 2004)

We introduce a technique based on algebraic topology for quantifying spatio-temporally chaotic dynamics. The technique is illustrated using the Gray-Scott and the FitzHugh-Nagumo models.

DOI: 10.1103/PhysRevE.70.035203 PACS number(s): 82.40.Bj, 05.45.Jn, 82.40.Ck, 89.75.Kd

Introduction. It is well established both numerically and experimentally that nonlinear systems involving diffusion, chemotaxis, and/or convection mechanisms can generate complicated time-dependent patterns. Specific examples include the Belousov-Zhabotinskii reaction [1–5], the Gray-Scott model [6,7], the oxidation of carbon monoxide on platinum surfaces [8], slime mold [9], the cardiac muscle [10–13] and excitable media [14–16]. Because this phenomenon is global in nature, obtaining a quantitative mathematical characterization that to some extent records or preserves the geometric structures of the complex patterns is difficult. In this Rapid Communication we propose a technique aimed at this problem. More precisely we show that using algebraic topology, in particular homology, we can measure Lyapunov exponents that imply the existence of spatial-temporal chaos and suggest a tentative step towards the classification and/or identification of patterns within a particular system.

Since the emphasis of this Rapid Communication is on the presentation of the technique, we have chosen to work with two well-studied systems: the 1-dimensional (1D) Gray-Scott model

$$u_t = d_1 u_{xx} - uv^2 + F(1-u),$$
$$v_t = d_2 v_{xx} + uv^2 - (F+k)v \tag{1}$$

on the interval $\Omega=[0,1.6]$ and the 2-dimensional (2D) FitzHugh-Nagumo system

$$u_t = \Delta u + \epsilon^{-1} u(1-u)\left(u - \frac{v+\gamma}{\alpha}\right),$$
$$v_t = u^3 - v \tag{2}$$

on the rectangular domain $\Omega=[0,80]\times[0,80]$. We use (1) to develop the geometric intuition behind our approach and thus restrict our computations to a single set of parameter values: $d_1=2\times10^{-5}$, $d_2=10^{-5}$, $F=0.035$, and $k=0.05632$ at which complicated spatio-temporal dynamics has been reported [6,7]. To demonstrate the potential of our technique and to emphasize that the method is dimension independent, we study (2) at $\alpha=0.75$, $\gamma=0.06$ and vary the parameter ϵ.

Since these are time-dependent problems, the simplest way to observe the dynamics of the patterns is to threshold the data, color the excited regions, and create movies. In the case of (1), each frame of the movie is 1D and hence the dynamics can be better viewed as a plot in the 2D space-time domain. Figure 1 shows a sample pattern generated in this fashion. An important point is that this thresholded movie provides the input data for the technique we are about to describe. Thus, in principle, this method can be applied in exactly the same manner to thresholded data produced from experimental as opposed to numerical data.

Excited space-time geometry. As indicated above, our goal is to understand and quantify the spatial and temporal geometry of patterns. For this purpose it is useful to think of the excited media as a subset of $\Omega\times[0,\tau]$, where the last direction represents time and τ is the length of the movie. If, as is the case in (1), Ω is 1D, then each colored pixel of Fig. 1 can be viewed as a 2D cube. Thus the excited media is represented by a set E in $\mathbb{R}^2$ consisting of a finite union of cubes. Let $V_{i,k}$ denote the cube corresponding to the pixel x_i for the kth frame of the movie, then $E=\{V_{i,k} \mid v(x_i,t_k) \geqslant 0.23\}$. Observe that, viewed as a finite collection of cubes, E provides a combinatorial representation of the excited media. At the same time E is a subset of $\Omega\times[0,\tau]$ that approximates the geometry of the excited media in both space and time.

Similar ideas apply to (2), for which Ω is 2D so that the elementary objects in space-time are 3-dimensional (3D) cubes. The excited media is represented by $E=\{V_{i,j,k} \mid u(x_i,y_j,t_k) \geqslant 0.9\}$.

In the next section we discuss how algebraic topology can be used to measure the complexity of the geometry of the patterns. Before doing so, recall that we are trying to quan-

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tify both the spatial structures of the patterns and how they change with time. Conceptually, the simplest way to do this is to compute the topology of each frame of the movie and then measure the change. Unfortunately, this approach cannot measure the global interactions between the fronts of the patterns that occur at different points in time. The other extreme is to consider the topology of E itself. However, if the dynamics of the original system is chaotic, then it is recurrent, and hence for large τ much of the structure should be redundant.

For these reasons we introduce the notion of a *time block* $T_{n,b}:=\{V_{i,k}\in E \mid n\leqslant k\leqslant n+b\}$. Figure 1 shows the time block $T_{1500,2000}$ for (1). Observe that $T_{n,0}$ represents the nth frame of the movie. For fixed b, $T_{n,b}$ captures the geometry of the pattern interactions over a given time range. We can see how this evolves by studying a sequence of time blocks of the form $\{T_{a(m-1),b} \mid m=1,2,\ldots,M\}$.

Computing homology. Algebraic topology is employed to measure the topological complexity of the excited patterns. In particular we make use of the fact that to any topological space X one can assign homology groups $H_i(X)$, $i=0,1,2,\ldots$ (see [17]). Clearly, this is not the venue in which to discuss homology theory, however, there are two issues that need to be considered: the geometric information that these groups contain and how they can be computed.

Returning to the very restricted setting of this Rapid Communication, for any time block $T_{n,b}$, $H_i(T_{n,b})\cong\mathbb{Z}^{\beta_i}$, where $\mathbb{Z}$ is the group of integers. The nonnegative integer β_i is called the ith Betti number of $T_{n,b}$. Due to the fact that $T_{n,b}\subset\mathbb{R}^{\dim(\Omega)+1}$, $\beta_i=0$ for $i>\dim(\Omega)$. Betti numbers give the following geometric information: β_0 equals the number of connected components that make up the space, β_1 indicates the number of holes (tunnels in 3D), and β_2 represents the number of cavities.

To compute the Betti numbers we make use of the fact that homology remains invariant under scaling and translation. For each $V_{i,k}\in E$, define $Q_{i,k}:=[i,i+1]\times[k,k+1]$ {in the case of (2) each $V_{i,j,k}\in E$ defines $Q_{i,j,k}:=[i,i+1]\times[j,j+1]\times[k,k+1]$}. Let $\mathbb{T}_{n,b}:=\{Q_{i,k} \mid V_{i,k}\in T_{n,b}\}$. Then $H_i(\mathbb{T}_{n,b})\cong H_i(T_{n,b})$. Because $\mathbb{T}_{n,b}$ is the union of unit cubes defined in terms of an integer lattice, it is a *cubical set*. Algorithms for the computation of the homology of cubical sets can be found in [18,19], and their implementation can be found at [20].

Topological results for Gray-Scott. As mentioned in the Introduction, we will use the existence of a positive Lyapunov exponent to conclude the existence of spatial-temporal chaos. This Lyapunov exponent will be measured by means of a time series of Betti numbers.

To produce a time series that incorporates the spatial structure, we computed the Betti numbers of various $\mathbb{T}_{n,b}$. More precisely, we computed $\{H_*(\mathbb{T}_{300(m-1),10\,000}) \mid m=1,2,\ldots,12\,000\}$ and hence obtained the Betti numbers $\beta_i(m)$ for $H_i(\mathbb{T}_{300(m-1),10\,000})$.

Our first observation was that $\beta_0(m)$ is piecewise constant taking on a limited number of fairly small values. However, the time series $B_{(300,10\,000)}:=\{\beta_1(m) \mid m=1,2,\ldots,12\,000\}$ proved to be quite interesting. A plot of the first 2000 points of this time series is indicated in the bottom picture of Fig. 1.

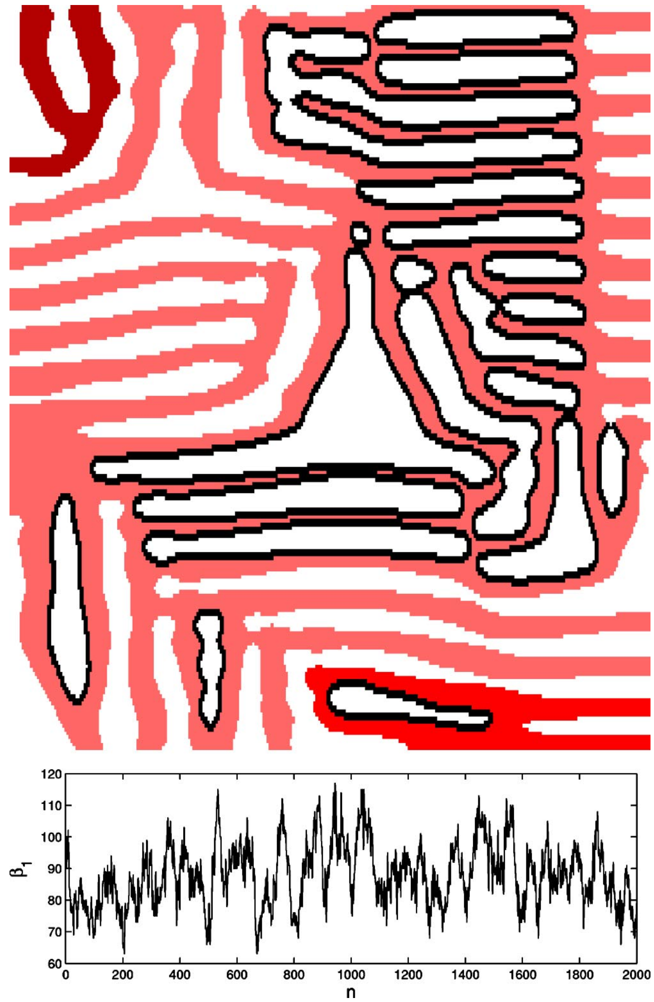

FIG. 1. (Color online) The top figure is the time block $T_{1500,2000}$ for (1). The black and gray (black and red) region indicates the evolution of the pattern of the excited media defined by $v\geqslant 0.23$. Observe that the black and gray (black and red) region decomposes into three connected components represented by three shades of gray (red); thus $\beta_0=3$. The black points are included to highlight the holes (cycles). There are twenty such holes and hence $\beta_1=20$. Consider the leftmost hole for example; it arises from the division of one hump into two humps which separate for some amount of time and then coalesce together at a later point in time. The bottom figure is a plot of the time series $\{\beta_1(m) \mid m=1,2,\ldots,2000\}$ of Betti numbers generated by such time blocks. This time series has a maximal Lyapunov exponent approximately equal to 0.037.

Using the algorithms in [21,22], we obtained a maximal Lyapunov exponent of approximately 0.037 for this time series, which confirms the existence of spatio-temporal chaos (see [6,7]).

The FitzHugh-Nagumo model. With the intuition developed in the previous example, we now turn to the 2D model (2). We numerically solved it using code of Barkley [23–25]. Again, dynamics of the patterns of the variable u is most easily observed by producing a movie of the thresholded data. Figure 2 shows some snapshots of such a movie at different values of the parameter ϵ. In particular, for $1/\epsilon$

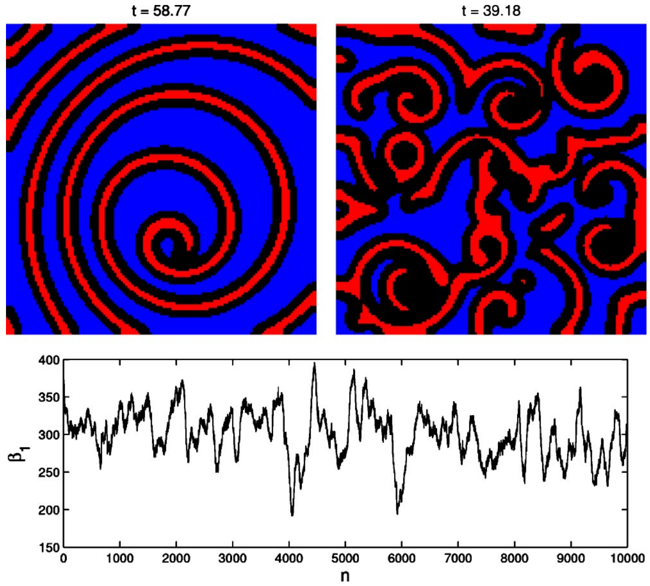

FIG. 2. (Color online) Wave patterns generated by (2). The light gray (red) region corresponds to excited points ($u \geqslant 0.9$), dark gray (blue) to the quiescent region ($u \leqslant 0.1$), and black to the reaction zone ($0.1 < u < 0.9$). In the top left figure we used $1/\epsilon = 14$ (in which case the pattern consists of a single spiral wave), and in the top right $1/\epsilon = 12$ was used. The bottom picture is a plot of the time series $\{\beta_1(m) \mid m = 1, 2, \ldots, 10\,000\}$ of Betti numbers for $1/\epsilon = 11.5$.

$\leqslant 12.5$ the movies indicate complicated spatial and temporal patterns.

Benchmark results. We feel it is important to compare our approach against the following more standard Lyapunov exponent computation. We fixed (i,j) such that $(x_i, y_j) = (11.4286, 21.4286)$ and produced a time series $\{u(x_i, y_j, t_k) \mid k = 0, \ldots, K\}$. We obtained estimates for the maximal Lyapunov exponents as indicated in Fig. 3. We obtained essentially the same result for several grid points (x_i, y_j).

From these computations we conclude that, for those values of ϵ at which the maximal Lyapunov exponent is positive, (2) exhibits temporally chaotic dynamics. However, it is important to observe that this computation completely ignores the spatial complexity of this system.

Topological results for FitzHugh-Nagumo. Just as in the Gray-Scott model, we again produce a time series by computing the Betti numbers of various time blocks $\mathbb{T}_{n,b}$. More precisely, we computed $\{H_*(\mathbb{T}_{10(m-1),1000}) \mid m = 1, 2, \ldots, 10\,000\}$ and hence obtained the Betti numbers $\beta_i(m)$ for $H_i(T_{10(m-1),1000})$.

Again $\beta_0(m)$ was piecewise constant taking on a limited number of fairly small values. Moreover, $\beta_2(m) \equiv 0$ so that there were no enclosed cavities in E. However, the time series $B_{(10,1000)} := \{\{\beta_1(m) \mid m = 1, 2, \ldots, 10\,000\}$ proved again to be chaotic. A typical plot is indicated in Fig. 2.

We computed the maximal Lyapunov exponent for the time series $B_{(10,1000)}$. Figure 3 provides a plot of the maximal Lyapunov exponent as a function of $1/\epsilon$. There are three important points to be made. The first is the near agreement between the ranges of ϵ on which the maximal Lyapunov exponents are positive and zero. This suggests computing the Lyapunov exponent from homological data is an acceptable approach. The second is that we can now conclude that the system exhibits *spatial-temporal chaotic* behavior. This follows from the fact that this chaotic time series is defined in terms of the Betti numbers β_1, since $\beta_1(m) \neq 0$ implies that the topology of $T_{10(m-1),1000}$ is nontrivial and $\beta_1(m) \neq \beta_1(m')$ implies that the topology of $T_{10(m-1),1000}$ differs from that of $T_{10(m'-1),1000}$. The fact that the Lyapunov expo-

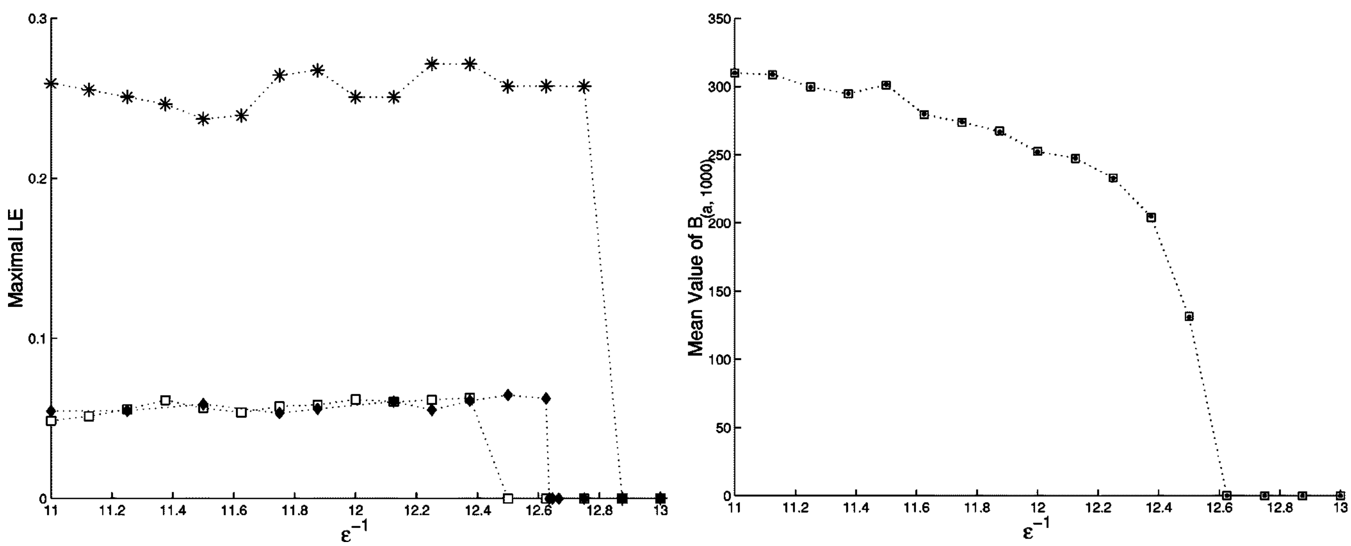

FIG. 3. Left: Maximal Lyapunov exponents, as a function of $1/\epsilon$, from the time series generated by fixing the point $(x_i, y_j) = (11.4286, 21.4286)$ in the domain and solving (2) for 30 000 time steps (stars). The diamonds and the squares are the Lyapunov exponents of time series of Betti numbers $B_{(10,1000)}$ computed using different initial conditions. For points where the Lyapunov exponent computation was not conclusive, the Lyapunov exponents were set to zero. Right: Mean values of the time series $B_{(10,1000)}$ used to compute the Lyapunov exponents in the left picture (squares), and the mean values of the time series $B_{100,1000} = \{\beta_1(m) \mid m = 1, 2, \ldots, 100\}$ (dots), as functions of $1/\epsilon$.

nent from the homological data goes to zero sooner than that computed from a single point can be explained by the fact that the latter measures temporal chaos only and the homological data measures spatial structures as well. Thus it is possible that the spatial-temporal chaos disappears before the purely temporal chaos does. The third point is the observation that, as in the case of a fixed (x_i, y_i), the maximal Lyapunov exponent appears to be essentially constant as a function of $1/\epsilon$ until it drops to zero. This implies that Lyapunov exponents do not provide a useful measurement for characterizing the value of ϵ at which the simulation is being performed. On the other hand, plotting the average value of β_1, as is done in Fig. 3, results in an almost monotone curve. Thus, in principle, by computing the average of the Betti numbers we can determine the parameter value ϵ of the simulation. Computing the average of the Betti numbers is much cheaper than computing the maximal Lyapunov exponent, because, as is indicated in Fig. 3, it can be computed with a shorter time series.

Computational comments. The above mentioned results depend upon the choice of a and b for the time blocks $T_{a(m-1),b}$. For the examples presented in this Rapid Communication, the choices $a=300$ and $b=10\,000$ for (1), and $a=10$ and $b=1000$ for (2) seem to be satisfactory. However, we cannot at this point in time suggest useful heuristics for a particular choice. The principal issues are as follows. If b is small, then β_1 is small. Since the Betti numbers are integers, this implies that we do not have enough significant figures to compute Lyapunov exponents. If b is large then the cost of computing $H_1(\mathbb{T}_{n,b})$ becomes impractical. Since the system is chaotic, choosing a too large results in decorrelation of subsequent Betti numbers. On the other hand, if a is too small the local change in the Betti numbers is insignificant. It should be noted that, for computing the mean value of the Betti numbers for (2), we were able to use $a=100$ because strong correlation is not necessary.

The typical running time for generating one of the 10 000 points time series used in Fig. 3 is about 12 CPU hours or 52 wall time hours in a Beowulf cluster with 30 Pentium 4, 2.4 GHz processors. On the other hand, each of the 100 points time series requires only 0.12 CPU hours or 0.5 wall time hours.

Conclusion. We have proposed the use of computational homology to measure the spatial-temporal complexity of patterns for systems that exhibit complicated spatial patterns. In addition we have shown that this technique can be used as a means of differentiating between patterns at different parameter values. Furthermore, although it is computationally expensive to measure spatial-temporal chaos, the computations necessary to do such discrimination are relatively cheap. One important feature of the proposed method is that it is fairly automated and can be applied to experimental data.

M.G. was partially supported by NSF Grant DMS 0107396, and by CAPES, Brazil. W.K. was partially supported by NSF Grant DMS 9973331. K.M. was partially supported by NSF Grant DMS 0107396. Computations were supported by the Center for Computational Molecular Science and Technology at the Georgia Institute of Technology and partially funded through a Shared University Research (SUR) grant from IBM and the Georgia Institute of Technology.

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