Self-Replication, Self-Destruction, and Spatio-Temporal Chaos in the Gray-Scott Model

Yasumasa NISHIURA[1]* and Daishin UEYAMA[2]

[1]*Laboratory of Nonlinear Studies and Computations, Research Institute for Electronic Science, Hokkaido University, Kita-ku, Sapporo 060-0812, Japan*
[2]*Department of Mathematical and Life Sciences, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8526, Japan*
E-mail: nishiura@aurora.es.hokudai.ac.jp, daishin@math.sci.hiroshima-u.ac.jp

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Abstract. A new geometrical understanding for the spatio-temporal chaos arising in the Gray-Scott model is presented. This is based on the interrelationship of global bifurcating branches of stationary patterns with respect to the supplying and removal rates contained in the model, especially their locations of saddle-node points and the Hopf bifurcation point of a constant state play a key role. It is possible to clarify the spatial structure of intermittent type of behavior by taking this point of view. At the onset point there exists a generalized heteroclinic cycle on the whole line and spatio-temporal chaos emerges by unfolding this cycle.

1. Introduction

Since early 90's, a variety of chemical patterns have been observed in chemical laboratories (KEPPER *et al.*, 1994; LEE *et al.*, 1994; LEE and SWINNEY, 1995), and among them, self-replicating patterns (SRP) and spatio-temporal chaos (STC) are spectacular examples. Self-replicating patterns have been also observed numerically (PEARSON, 1993; REYNOLDS *et al.*, 1994; PETROV *et al.*, 1994; RASMUSSEN *et al.*, 1996) for the following Gray-Scott model (GRAY and SCOTT, 1984):

$$\begin{cases} \dfrac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1-u), \\ \dfrac{\partial u}{\partial t} = D_u \nabla^2 u + uv^2 - (F+k)v \end{cases} \tag{1}$$

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where u and v are concentrations of the chemical materials U and V, respectively, D_u and D_v the diffusion coefficients, F the in-flow rate of U from outside, $F + k$ the removal rate of v from reaction field. Note that $(u, v) = (1, 0)$ is a stable homogeneous state independent of (k, F). Several interesting analytical works for Eq. 1 have appeared recently: For instance, construction of single-spot solution and its stability has been done by REYNOLDS *et al*. (1997) with the aid of formal matched asymptotic analysis, which is closely related to the splitting phenomenon; A rigorous analysis concerning the existence and stability of steady single pulse as well as nonexistence of traveling pulses has been done quite recently by DOELMAN *et al*. (1997, 1998). Despite these works, we don't know yet how and why the transitions occur from one dynamics to another, especially what kind of geometrical structure causes SRP and STC. As for SRP, it was found recently by (NISHIURA and UEYAMA, 1999) that a hierarchy structure of saddle-node bifurcations is responsible for SRP. Such a structure not only explains a driving mechanism of SRP, but also locates the onset point of it. The model system treated by them is Eq. (1), however the geometrical structure extracted from it has a universal character independent of the systems. It has been illustrated for other problems (see, for instance, ARGENTINA *et al*. (1997)) that such a geometrical view point is quite useful to understand the dynamic transition.

The aim of this paper is of two-fold. One is to clarify the *onset point* of spatio-temporal chaos arising in the Gray-Scott model. The same spirit as in NISHIURA and UEYAMA (1999), i.e., a geometrical structure of global bifurcation diagram of steady states, plays a key role to give such an criterion, in fact, the minimum (denoted later by $k_{\min}$) of saddle-node points of steady branches gives the onset point. The other is to understand the detailed mechanism which drives a chaotic behavior from pattern formation point of view, namely we show the existence of *heteroclinic cycle* at the onset point of STC, and STC emerges by unfolding it in a parameter space. In other words we would like to understand the spatio-temporal chaos (STC) in a constructive way with keeping its spatial character rather than projecting the infinite dimensional dynamics to an effective finite dimensional one and computing the statistical quantities.

There are several types of STC's for the Gray-Scott model depending on parameter values, however we focus on the representative case like Fig. 1 called *the STC of static type* where the quasi-steady state is observed during the STC process. Looking closely at the sequence of snapshots of Fig. 1, one can see the cycle: homogeneous state $\rightarrow$ (1, 0) $\rightarrow$ periodic steady state $\rightarrow$ homogeneous state, which corresponds to the heteroclinic cycle mentioned above. Finally we assume that the system size is large compared with the unit size of steady state, otherwise diffusivity dominates the system.

2. Phase Diagram of PDE Dynamics in 1D

Starting from a spiky localized initial data, the Gray-Scott model displays a variety of dynamics as in Fig. 2. The main feature of the associated ODE of Eq. (1) has a Bogdanov-Takens (BT)-point together with a stable critical point $(u, v) = (1, 0)$. BT-point is a singularity of codim 2 and located at $(k, F) = (1/16, 1/16)$ where saddle-node and Hopf bifurcations merge there in 2-dimensional parameter space (k, F) (see the caption in Fig. 2). Before the saddle-node bifurcation, (1, 0) is the only equilibrium point and globaly stable, and hence the system has an excitable character. We denote the two constant states

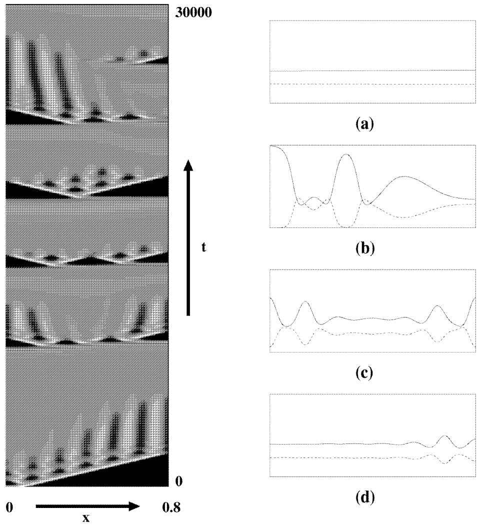
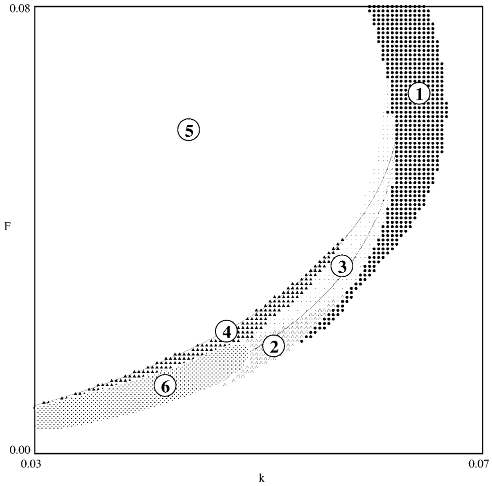


Fig. 1. Spatial-temporal chaos of static type for $D_u = 2 \times 10^{-5}$, $D_v = 10^{-5}$, $F = 0.035$, $k = 0.05632$ and L(= width of interval) = 0.8. The snapshots indicate the existence of heteroclinic cycle.

born from the saddle-node bifurcation by P and Q where P is a unstable node and Q is a saddle. P recovers its stability via Hopf bifurcation as k is decreased. As for PDE dynamics, there are at least five different regimes in (k, F)-space (see Fig. 2): standing pulse, traveling pulse, self-replication patterns, traveling front, and spatio-temporal chaos, respectively. Each transition from one regime to another is sharp and the main objective is to clarify the mechanisms of such transitions, especially to chaotic one. It turns out that a global interrelation among the branches of the ordered states becomes important, in particular, the relation between locations of saddle-node points of them and the Hopf bifurcation point of the constant state P becomes crucial to understand such a transition.

3. Spatio-Temporal Chaos

There are many routes to chaos like period-doubling, breakdown of torus, intermittency and so on. The STC of static type maybe classified as an intermittency type I (see, for instance, OTTO (1993), however, from pattern formation point of view, this does not explain much about the spatial aspect of intermittent behavior, for instance, which patterns the orbit itinerate. In this section we first present a new criterion for the onset of spatio-temporal chaos based on an interrelationship among global bifurcation branches of ordered states and its influence over the dynamics as an aftereffect. Second, by taking this view point, we can understand the detailed mechanism of the spatio-temporal chaos from pattern formation view point without projecting the whole dynamics to an effective finite dimensional space. In fact we find basic building blocks of pattern dynamics participating in the spatio-temporal chaos, and the above view point allows us to know how each block contributes



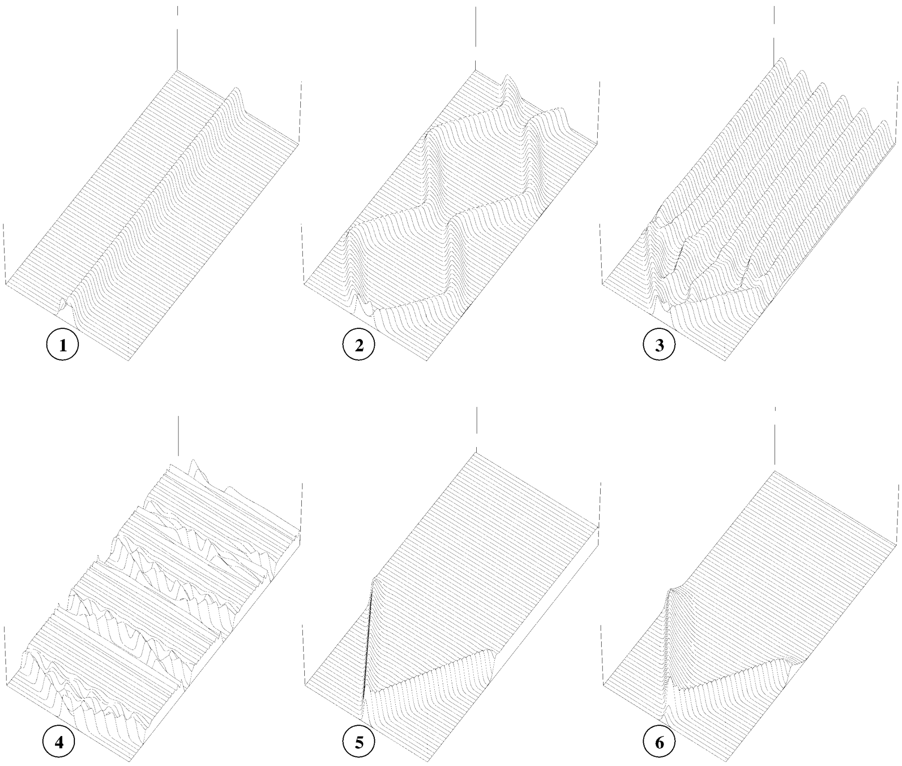


Fig. 2. The boundary condition is of Neumann type. Region 1: Standing pulse, region 2: Traveling pulse, region 3: Self-replicating patterns, region 4: Spatio-temporal chaos, region 5: Traveling front, region 6: Annihilation. The upper (resp. lower) curve in (k, F)-space denotes the Hopf-line for P (resp. the saddle-node-line).

to form chaotic behavior. It turns out that three building block dynamics form a heteroclinic cycle at the onset point in infinite dimensional space, and the parameter, say k, is decreased, then STC emerges.

4. Pattern-Switching Processes and Heteroclinic Cycles

There are three basic dynamics participating the STC of static type.

1. *ODE dynamics*: Switching from the homogeneous state P to the background state (1, 0). There exists a $k = k_{\text{Hopf}}$ such that P is unstable for $k > k_{\text{Hopf}}$ and the homogeneous limit cycle emanating at $k = k_{\text{Hopf}}$ is unstable and exists only for $k < k_{\text{Hopf}}$ (subcritical), hence P is taken over by the background state (1, 0) by homogeneous perturbation.
2. *SRP dynamics*: Switching from (1, 0) to an steady state. This is brought by SRP dynamics, i.e., when a localized perturbation of finite amplitude is added to (1, 0), then SRP of front type as in Fig. 4 invades into (1, 0) and spatially periodic structure is formed after the front.
3. *Self-destruction*: Switching from a steady state to the homogeneous state P. Suppose there exists a saddle-node branch of an ordered state, say a stationary pattern as in Fig. 3 and the associated unstable manifold is connnected to an homogeneous state. Then the corresponding aftereffect displays a self-destruction, namely, an ordered state persists for a while, the duration of which depends on how close the parameter value to the saddle-node bifurcation point, but eventuallly decays to the constant state.

These three processes can be regarded as *heteroclinic orbits* on a whole line, for instance, the second one is a heteroclinic orbit connecting the background state (1, 0) to a spatially periodic pattern as in Fig. 4.

Moreover it should be noted that these three connections constitute formally a *heteroclinic cycle* on **R** as in Fig. 5 provided that all the connections occur exactly at the same parameter value. Such an miraculous coincidence does not seem to occur generically, however it turns out that such a tuning is possible by controlling two parameters k and F. Here we loosely describe how an orbit makes a cycle locally in space starting from the

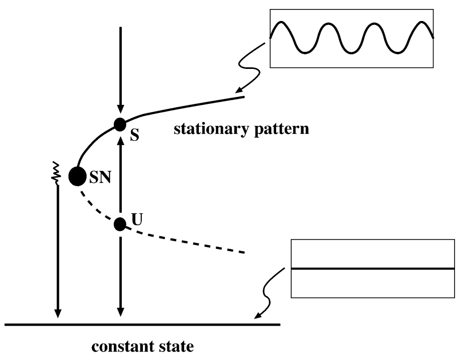


Fig. 3. The saddle-node point induces a self-destruction if the unstable manifold of U is connected to the constant state.

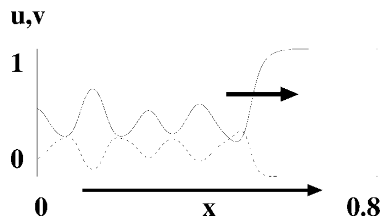


Fig. 4. The stationary pattern is obtained through the replication process.

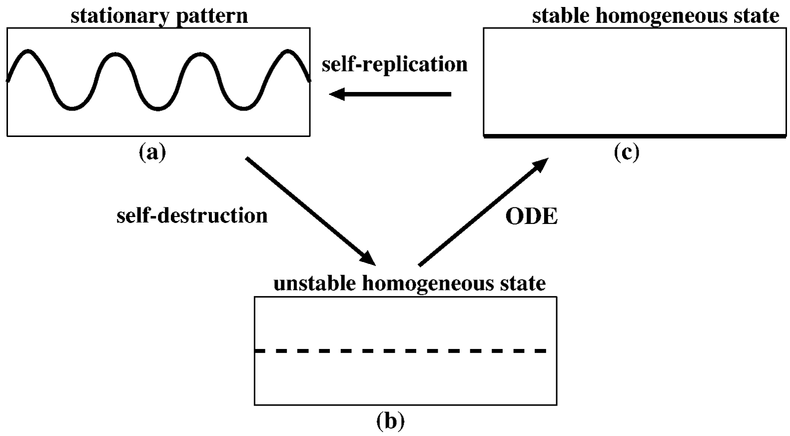


Fig. 5. Heteroclinic cycle on the infinite line.

unstable constant state P through three switching processes (see Figs. 1 and 5). Suppose a small perturbation of long wavelength is added to P, initial phase difference is amplified and the solution goes to (1, 0) on phase-gaining part of the interval and the remaining part, which is still far from (1, 0), becomes a trigger of invading front into (1, 0) followd by an spatially periodic steady state. Finally this ordered state decays to the homogeneous state P through the destruction process, which completes the cycle.

5. Unfolding the Heteroclinic Cycle—Spatio-Temporal Chaos of Static Type

Each process of dynamics in the previous section does not show any chaotic behavior by itself, however if they are combined together appropriately, the resulting one becomes chaotic in space and time. The main idea is to unfold the heteroclinic cycle in infinite dimensional space by adjusting the parameters in such a way that the orbit itinerate this cycle chaotically in space and time. This is apparently a reminiscent of the homoclinic tangling in finite dimensional dynamical system.

We shall now discuss how the dynamics is controlled by the global arrangement of branches. STC of this type is typically observed in the area 4 of Fig. 2 and the time-evolution at $F = 0.035$ and $k = 0.05632$ is given by Fig. 1. On the other hand, for slightly larger F, say $F = 0.04$, we do not observe any chaotic pattern. To understand this difference and the onset of STC, we draw two schematic global bifurcation diagrams of stationary patterns for each F (see Fig. 6). The main difference of two diagrams (a) and (b) of Fig. 6 is the *order* of two quantities k_{min} and k_{Hopf}, namely $k_{\mathrm{min}} < k_{\mathrm{Hopf}}$ for (a) and $k_{\mathrm{min}} > k_{\mathrm{Hopf}}$ for (b). Here the k_{min} is the smallest value of k among the locations of saddle-node points of the steady states. The value k_{min} is computable with the aid of AUTO software, since, in most cases, it coincides as in Fig. 6 with the SN-point of stationary branch which is the continuation of the final state after self-replication, and the k_{Hopf} is the Hopf bifurcation point of the homogeneous state P. The k_{Hopf}-line is explicitly calculated and becomes a monotone function of F (the solid line in Fig. 7). The k_{min} -line is much harder to compute,

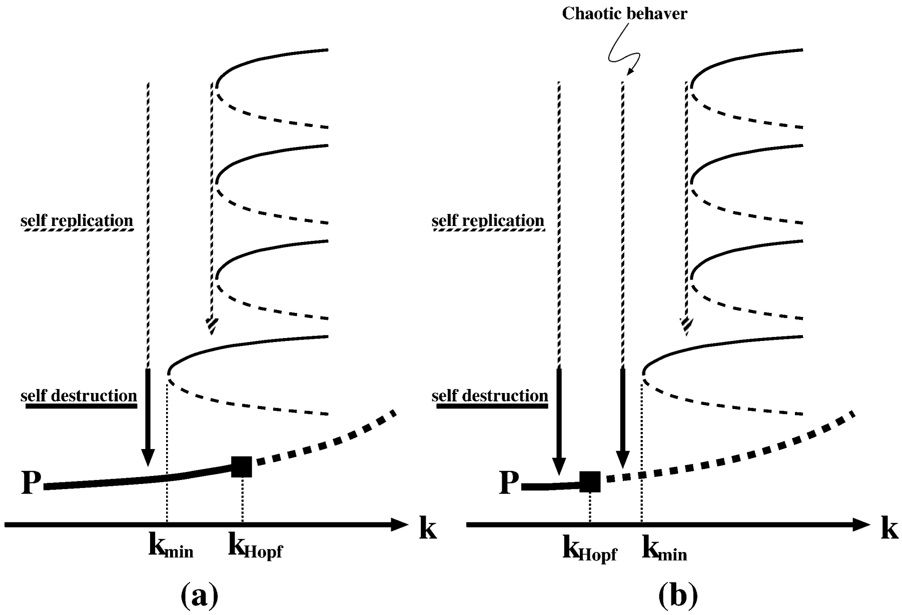


Fig. 6. (a) The schematic bifurcation diagram for $F = 0.04$. After self-destruction, the orbit settles down to the stable homogeneous state P, (b) For $F = 0.035$, the order of two quantities k_{min} and k_{Hopf} is reversed and if k belongs to the interval $(k_{\mathrm{Hopf}}, k_{\mathrm{min}})$, the orbit itinerates in a chaotic way.

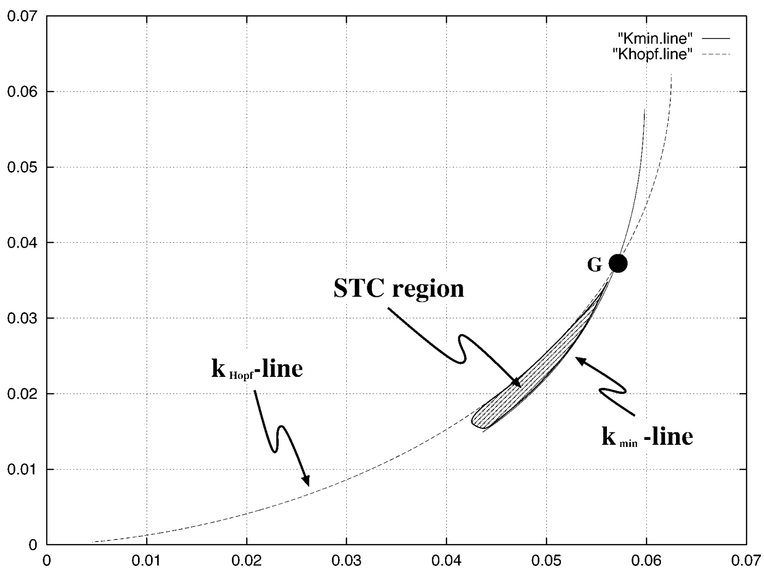


Fig. 7. Numerical plots of k_{min} and k_{Hopf}. Both are monotone functions of F. There exists a unique intersecting point G from which the STC region emerges.

since it is a locus of saddle-node points of stationary branches depending on F. It turns out that the function $k_{\min}$(F) is also monotone, but less steep than $k_{\mathrm{Hopf}}(F)$ (the dotted line in Fig. 7). Therefore there exists a unique intersecting point G in (k, F)-space as in Fig. 7, and the order of these quantities are reversed at G. The region below G sandwitched by two curves $k_{\min}$ and k_{Hopf} is called *STC* (*spatio-temporal chaos*) *region* where we observe spatio-temporal chaos. It should be noted that *the curve* $k_{min}(F)$ *perfectly fits the right boundary of STC region 4* in Fig. 2, which reveals the nature of the transition boundary. In other words, once we know the location of $k_{\min}(F)$, we can *predict* the onset of STC in the parameter space.

Heteroclinic cycle can be constructed at least formally at any point on the right boundary of STC-region (i.e., $k = k_{\min}$(F)), and STC is observed as a result of unfolding of this cycle. Heteroclinic cycle at $k = k_{\min}$ consists of three parts (see Fig. 5): P to (1, 0), (1, 0) to stationary pattern, and the destruction process to P. Note that the connection between the unstable part of the saddle-node branch and the homogeneous state P still persists even if P loses its stability. When k belongs to the interval $k_{\mathrm{Hopf}} < k < k_{\min}$ (see Fig. 6(b)), the spatio-temporal chaos is invoked in the following way (see Fig. 1). A spatially periodic pattern is formed after the SRP process initiated by the initial trigger, but it only lasts for a while and approaches P due to the aftereffect of the connection to P. Since P is unstable, the orbit bounces except that it accidentally lies on the stable manifold of P. Recalling that the intial data is a localized spiky perturbation of finite amplitude, the process of approaching P does not occur uniformly on the interval I as is shown in Fig. 1; the solution is close to P on some portion of the interval, then the ODE dynamics dominates there, and therefore it reaches quickly background state. Once such an background region is formed, the SRP wave (or modulating front) starts to propagates into this region and (1, 0)-state is taken over by a periodic structure, however the periodic structure after the front survive only temporalily in this parameter regime as before, hence it eventually disappear and becomes close to homogeneous state P again. In this manner the orbit does not settle down to any ordered state and makes a chaotic cycle.

On the other hand, if F is above G (for instance $F = 0.04$), the self-destruction process also occurs for $k < k_{\min}$, however no heteroclinic cycle is formed since P is stable. Summarizing the above discussions, the unique intersecting point

$$k_{\min} = k_{\mathrm{Hopf}}$$

characterizes the vertex point G of the STC region (denoted by black triangle region) in Fig. 2, and the boundaries of STC region coincides with the two curves $k = k_{\min}(F)$ (lower boundary) and $k = k_{\mathrm{Hopf}}(F)$ (upper boundary). We thus conclude that STC region is completely characterized by two quantities $k_{\min}$ and k_{Hopf}.

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