Turing instability for a two dimensional semi-discrete Gray-Scott system

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Abstract: This paper is concerned with the spatial patterns of the Gray-Scott system which describes a general two-variable kinetic model that represents an activator-substrate scheme, where the space is discrete in two dimensions with the periodic boundary conditions and the time is continuous. Furthermore conditions for producing Turing instability of a general semi-discrete system are obtained through linear stability analysis and this conclusion is applied to the semi-discrete G-S model. Then in the Turing instability region of semi-discrete G-S model, we perform a series of numerical simulations which shown that this system can produce some new Turing patterns such as striped, spotted and lace-liked patterns in the Turing instability region. In particular, the observation of Turing patterns are reported, as a control parameter is varied, from a spatially uniform state to a patterned state. It suggests that the values of parameters make a great impact on Turing patterns.

Key–Words: Semi-discrete; Gray-Scott model; Turing instability; Turing pattern; Diffusion; Pattern formation

1 Introduction

The Turing system involves a pair of partial differential equations, and represents the time course of reacting and diffusing chemicals. It can evolve spontaneously into a spatially heterogeneous stationary pattern from an initially uniform distribution [1]. Without diffusion, the local reaction of the two substances is stable and converges to the equilibrium, however, with diffusion, the uniform steady state is unstable. This spontaneous emergence of a spatially heterogeneous pattern is referred to as "the Turing instability". This mechanism suggests that the reaction of a small number of chemicals and their random diffusion can create stable non-uniform patterns in a perfectly homogeneous field [2]. It is well known that Turing patterns are very important for a reaction-diffusion system. It has been proposed as mechanisms for biological pattern formation in embryological and ecological context [3]. All such works are based on the pioneering work of Turing [1].

As everyone knows, the Gray-Scott model (G-S model) [4,5] is a critical reaction-diffusion system. It is a variant of the autocatalytic model of glycolysis first proposed by Selkov [6]. After proper modulating and including diffusion for convenience to illustrate Turing instability with discrete space, the kinetic equations for the reactions can be written as [7]:

$$\begin{cases} u'(t) = -uv^2 + F(1-u) + d\nabla^2 u, \\ v'(t) = uv^2 - (F+k)v + \nabla^2 v. \end{cases} \quad (1)$$

Here, u and v represent the concentrations of the chemical materials U and V, respectively, F is the flow rate, k is a decay constant of the activator. The ratio of diffusivity $d = \frac{D_u}{D_v}$, D_u and D_v are the diffusion constants for the two species.

In the research of pattern formation in the G-S model, a major development was performed by Pearson [08], in his paper, there were 12 categories patterns described for the G-S model, but only one of them is covered in the Turing region. Lee [7] reported their experiments in a ferro-cyanide-iodate-sulfite reaction which showed strong qualitative agreement with the self-replication regimes in simulations of [8]. Moreover, those same experiments led to the discovery of other new patterns, such as annular patterns emerging from circular spots see [9]. More detailed description about the G-S model can be found in contexts [10,11,12,13,14,15,16].

However, the G-S model with discrete space was caused little attention at present. Meanwhile, in 1957 [17], the first semi-discrete approach was put forward by Beverton and Holt in their construction of a discrete-time model analogous to the continuous-time logistic model on the basis of a semi-discrete model. Since then, a large body of literature has proposed semi-discrete models in almost every field of the life science: population dynamics and ecology, plant pathology, epidemiology, medicine, etc. From these, it can be seen that the research about semi-discrete system is of significance. With a difference, we care about the G-S model with discrete space.

Now, there comes a problem. Can the discrete-space G-S system produce Turing instability? If it can, what difference from a continuous one? In this paper, we will study the Turing instability of a two-dimensional semi-discrete G-S model and carry out a series of simulations. This paper is organized as following: in the next section ,we demonstrate the general theory of Turing instability for a semi-discrete system by using linearized technique.The conditions of Turing instability will be obtained. In Section 3 ,a semi-discrete G-S model will be introduced and the conditions of Turing instability via linear stability analysis will be achieved. In the following Section 4, a series of numerical simulations will be given for the semi-discrete G-S system with different parameters. kinds of Turing patterns can emerge in the Turing instability region, such as striped, spotted and lace-liked patterns. We can recognize that the varying of control parameters play an important role in pattern structure. Conclusions are drawn in Section 5.

2 Turing Instability for the semi-discrete System

Similar to [19], in this section, we firstly consider Turing instability for a general semi-discrete reaction-diffusion system

$$\begin{cases} u'_{ij}(t) = \gamma f(u_{ij}(t), v_{ij}(t)) + \nabla^2 u_{ij}(t), \\ v'_{ij}(t) = \gamma g(u_{ij}(t), v_{ij}(t)) + d\nabla^2 v_n^{ij}(t) \end{cases} \tag{2}$$

with the periodic boundary conditions

$$\begin{cases} u_{i,0}(t) = u_{i,m}(t), \\ u_{i,1}(t) = u_{i,m+1}(t), \\ u_{0,j}(t) = u_{m,j}(t), \\ u_{1,j}(t) = u_{m+1,j}(t) \end{cases} \tag{3}$$

and

$$\begin{cases} v_{i,0}(t) = v_{i,m}(t), \\ v_{i,1}(t) = v_{i,m+1}(t), \\ v_{0,j}(t) = v_{m,j}(t), \\ v_{1,j}(t) = v_{m+1,j}(t) \end{cases} \tag{4}$$

for $i,j \in \{1,2,\cdots,m\} = [1,m]$ and $t \in R^+ = [0,\infty)$, where m is a positive integer,

$$\begin{aligned} \nabla^2 u_{ij}(t) &= u_{i+1,j}(t) + u_{i,j+1}(t) \\ &+ u_{i-1,j}(t) + u_{i,j-1}(t) - 4u_{ij}(t) \end{aligned} \tag{5}$$

and

$$\begin{aligned} \nabla^2 v_{ij}(t) &= v_{i+1,j}(t) + v_{i,j+1}(t) \\ &+ v_{i-1,j}(t) + v_{i,j-1}(t) - 4v_{ij}(t). \end{aligned} \tag{6}$$

With no spatial variation u and v satisfy

$$\begin{cases} u'_{ij}(t) = \gamma f(u_{ij}(t), v_{ij}(t)), \\ v'_{ij}(t) = \gamma g(u_{ij}(t), v_{ij}(t)). \end{cases} \tag{7}$$

Suppose that (u^*, v^*) is the steady state of (7) and let

$$w_{ij}(t) = \begin{pmatrix} u_{ij}(t) - u^* \\ v_{ij}(t) - v^* \end{pmatrix} = \begin{pmatrix} x_{ij}(t) \\ y_{ij}(t) \end{pmatrix}.$$

The linearized form of (7) is then

$$\begin{aligned} &w'_{ij}(t) = \gamma A w_{ij}(t), \\ &A = \begin{bmatrix} f_u & f_v \\ g_u & g_v \end{bmatrix}_{(u^*,v^*)} \end{aligned} \tag{8}$$

which has the eigenvalue equation

$$\lambda^2 - \gamma (f_u + g_u) \lambda + \gamma^2 (f_u g_v - f_v g_u) = 0. \tag{9}$$

Linear stability, that is $\mathrm{Re}\lambda < 0$, is guaranteed if

$$\begin{aligned} &\mathrm{trA} = \mathrm{f_u} + \mathrm{g_v} < 0, \\ &|A| = f_u g_v - f_v g_u > 0. \end{aligned} \tag{10}$$

Now consider the system (2) and again linearize about the stead state, to get

$$\begin{aligned} &w'_{ij}(t) = \gamma A w_{ij}(t) + D\nabla^2 w_{ij}(t), \\ &D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \end{aligned} \tag{11}$$

with the periodic boundary conditions

$$\begin{cases} w_{i,0}(t) = w_{i,m}(t), \\ w_{i,1}(t) = w_{i,m+1}(t), \\ w_{0,j}(t) = w_{m,j}(t), \\ w_{1,j}(t) = w_{m+1,j}(t). \end{cases} \tag{12}$$

In order to study instability of (11), we firstly consider eigenvalues of the following equation

$$\nabla^2 X_{ij} + \mu X_{ij} = 0, \tag{13}$$

with the periodic boundary conditions

$$\begin{cases} X_{i,0} = X_{i,m}, \\ X_{i,1} = X_{i,m+1}, \\ X_{0,j} = X_{m,j}, \\ X_{1,j} = X_{m+1,j}. \end{cases} \quad (14)$$

In view of [18], the eigenvalue problem (13)-(14) has the eigenvalues

$$\mu_{l,s} = 4\left(\sin^2\frac{(l-1)\pi}{m} + \sin^2\frac{(s-1)\pi}{m}\right) = k_{ls}^2 \text{ for } l,s \in [1,m].$$

Then respectively taking the inner product of (2) with the corresponding eigenfunction X_{ts}^{ij} of the eigenvalue $\lambda_{t,s}$, we see that

$$\begin{cases} \sum_{i,j=1}^{m} X_{ls}^{ij} x'_{ij} = f_u \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij} \\ \quad + f_v \sum_{i,j=1}^{m} X_{ls}^{ij} y_{ij} + \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^2 x_{ij}, \\ \sum_{i,j=1}^{m} X_{ts}^{ij} y'_{ij} = g_u \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij} \\ \quad + g_v \sum_{i,j=1}^{m} X_{ls}^{ij} y_{ij} + D_2 \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^2 y_{ij}. \end{cases} \quad (15)$$

Let

$$U(t) = \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij},$$

$$V(t) = \sum_{i,j=1}^{m} X_{ts}^{ij} y_{ij}$$

and use the periodic boundary conditions (12) and (14), then we have

$$\begin{cases} U'(t) = \gamma f_u U(t) + \gamma f_v V(t) - k_{ls}^2 U(t), \\ V'(t) = \gamma g_u U(t) + \gamma g_v V(t) - d k_{ls}^2 V(t) \end{cases}$$

or

$$\begin{cases} U'(t) = \left(\gamma f_u - k_{ls}^2\right) U(t) + \gamma f_v V(t), \\ V'(t) = \gamma g_u U_n + \left(\gamma g_v - d k_{ls}^2\right) V(t). \end{cases}$$

Which has the eigenvalue equation

$$\lambda^2 + \left[k_{ls}^2 (1+d) - \gamma (f_u + g_u)\right] \lambda + h\left(k_{ls}^2\right), \quad (16)$$

where

$$h\left(k_{ls}^2\right) = d k_{ls}^4 - \gamma (d f_u + g_v) k_{ls}^2 + \gamma^2 |A|. \quad (17)$$

To guarantee the instability of (2), the instability can happen either if the coefficient of λ in (16) is negative,or if $h(k_{ls}^2) < 0$ for $k_{ls}^2 \in [0,8]$. Since $f_u + g_v < 0$ and $k_{ls}^2 > 0$ and $d \gg 1$, the coefficient of λ is positive. Thus, the only way $Re(\lambda) > 0$ can be positive if $k_{ls}^2 < 0$ for some k_{ls}^2, which is necessary but not sufficient for $Re(\lambda) > 0$. So the condition of instability of (2) is $h(k_{ls}^2) < 0$.

So the conditions of Turing instability

$$\begin{cases} \mathrm{trA} = \mathrm{f_u} + \mathrm{g_v} < 0, \\ |A| = f_u g_v - f_v g_u > 0, \\ h\left(k_{ls}^2\right) < 0. \end{cases}$$

are attained.

3 The semi-discrete Gray-Scott model

Now, we consider the G-S model with discrete space:

$$\begin{cases} u'_{ij}(t) = -u_{ij}(t) v_{ij}^2(t) + F(1 - u_{ij}(t)) \\ \qquad + d\nabla^2 u_{ij}(t), \\ v'_{ij}(t) = u_{ij}(t) v_{ij}^2(t) - (F+k) v_{ij}(t) \\ \qquad + \nabla^2 v_{ij}(t), \end{cases} \quad (18)$$

with the periodic boundary conditions of

$$\begin{cases} u_{i,0}(t) = u_{i,m}(t), \\ u_{i,1}(t) = u_{i,m+1}(t), \\ u_{0,j}(t) = u_{m,j}(t), \\ u_{1,j}(t) = u_{m+1,j}(t) \end{cases}$$

and

$$\begin{cases} v_{i,0}(t) = v_{i,m}(t), \\ v_{i,1}(t) = v_{i,m+1}(t), \\ v_{0,j}(t) = v_{m,j}(t), \\ v_{1,j}(t) = v_{m+1,j}(t) \end{cases}$$

for $i,j \in \{1,2,\cdots,m\} = [1,m]$ and $t \in R^+ = [0,\infty)$, where m is a positive integer. Laplace's operators are

$$\nabla^2 u_{ij}(t) = u_{i+1,j}(t) + u_{i,j+1}(t) + u_{i-1,j}(t) + u_{i,j-1}(t) - 4u_{ij}(t)$$

and

$$\nabla^2 v_{ij}(t) = v_{i+1,j}(t) + v_{i,j+1}(t) + v_{i-1,j}(t) + v_{i,j-1}(t) - 4v_{ij}(t).$$

In order to find the Turing instability region of the G-S model, we first analysis the model with no spatial variation, u and v satisfy:

$$\begin{cases} u'_{ij}(t) = -u_{ij}(t)v_{ij}^2(t) + F(1 - u_{ij}(t)), \\ v'_{ij}(t) = u_{ij}(t)v_{ij}^2(t) - (F + k)v_{ij}(t). \end{cases} \quad (19)$$

Clearly, the above system exhibits three possible steady states with $P_0 = (u_R, v_R) = (1, 0), P_1 = (u_B, v_B)$, and $P_2 = (u_I, v_I)$, where

$$u_B = \frac{1}{2}\left[1 - \sqrt{1 - \frac{4(F+k)^2}{F}}\right],$$
$$v_B = \frac{F}{2(F+k)}\left[1 + \sqrt{1 - \frac{4(F+k)^2}{F}}\right],$$
$$u_I = \frac{1}{2}\left[1 + \sqrt{1 - \frac{4(F+k)^2}{F}}\right],$$
$$v_I = \frac{F}{2(F+k)}\left[1 - \sqrt{1 - \frac{4(F+k)^2}{F}}\right]$$

and

$$1 - \frac{4(F+k)^2}{F} \geq 0.$$

The state P_0 is always linearly stable, for the other two states, we calculate the eigenvalues of the Jacobian matrix A to examine the stability, where

$$A = \begin{bmatrix} -v_*^2 - F & -2u_*v_* \\ v_*^2 & 2u_*v_* - (F+K) \end{bmatrix}$$

(with index * representing B or I), obtaining

$$\text{tr}A = -v_*^2 + k$$

and

$$|A| = (F+k)(v_*^2 - F).$$

We find that the state P_2 is always unstable because $\text{tr}A > 0$ and $|A| \leq 0$, moreover, when

$$1 - \frac{4(F+k)^2}{F} = 0,$$

$$v_I = \sqrt{F}$$

and $|A| = 0$, the system occurs the saddle-node bifurcation, that is

$$F_{SN} = \frac{1}{8}\left[1 - 8k \pm \sqrt{1 - 16k}\right].$$

The state P_1, on the other hand, may be stable. Next, we shall refer to this state. One finds that this state exhibits a Hopf bifurcation curve from the condition $\text{tr}A = 0$. Inserting $P_2(u_B, v_B)$ we find

$$F_H = \frac{1}{2}\left[\sqrt{k} - 2k - \sqrt{k(1 - 4\sqrt{k})}\right].$$

Below the $Hopf$ bifurcation curve $\text{tr}A = k - v_B^2 > 0$, and the state P_1 is unstable. More details about computation refer to [15].

Let

$$w_{ij}(t) = \begin{bmatrix} u_{ij}(t) - u_B \\ v_{ij}(t) - v_B \end{bmatrix} = \begin{bmatrix} x_{ij}(t) \\ y_{ij}(t) \end{bmatrix}$$

The linearized form of (19) is then

$$w'_{ij}(t) = Aw_{ij}(t),$$
$$A = \begin{bmatrix} -v_B^2 - F & -2u_Bv_B \\ v_B^2 & 2u_Bv_B - (F+K) \end{bmatrix}$$

Then consider the full reaction diffusion system of (19) and again linearize about the steady state, to get

$$w'_{ij}(t) = Aw_{ij}(t) + D\nabla^2 w_{ij}(t)$$

and

$$D = \begin{bmatrix} d & 0 \\ 0 & 1 \end{bmatrix}$$

with the periodic boundary conditions (12).

In order to study instability of (18),we firstly consider eigenvalues of the following equation

$$\nabla^2 X_{ij} + \mu X_{ij} = 0,$$

with the periodic boundary conditions

$$\begin{cases} X_{i,0} = X_{i,m}, \\ X_{i,1} = X_{i,m+1}, \\ X_{0,j} = X_{m,j}, \\ X_{1,j} = X_{m+1,j}. \end{cases}$$

Then we respectively take the inner product of (18) with the corresponding eigenfunction X_{ls}^{ij} of the eigenvalue $\lambda_{l,s}$, then

$$\begin{cases} \sum_{i,j=1}^{m} X_{ls}^{ij} u_{ij}^{'} = -(F+v_B^2) \sum_{i,j=1}^{m} X_{ls}^{ij} u_{ij} \\ \quad - 2u_B v_B \sum_{i,j=1}^{m} X_{ls}^{ij} v_{ij} \\ \quad + d \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^2 u_{ij}, \\ \sum_{i,j=1}^{m} X_{ls}^{ij} v_{ij}^{'} = v_B^2 \sum_{i,j=1}^{m} X_{ls}^{ij} u_{ij} \\ \quad + (F+k) \sum_{i,j=1}^{m} X_{ls}^{ij} v_{ij} \\ \quad + \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^2 v_{ij}. \end{cases}$$

Let

$$U(t) = \sum_{i,j=1}^{m} X_{ls}^{ij} u_t^{ij}$$

and

$$V(t) = \sum_{i,j=1}^{m} X_{ls}^{ij} v_t^{ij}.$$

Then use the periodic boundary conditions (3) , (4) and Abel transform, thus it follows that

$$\begin{cases} U^{'}(t) = -(F+v_B^2)U(t) - 2u_B v_B V(t) \\ \qquad - d k_{ls}^2 U(t), \\ V^{'}(t) = v_B^2 U(t) + (F+k)V(t) \\ \qquad - k_{ls}^2 V(t), \end{cases}$$

which has the eigenvalue equation

$$\lambda^2 + [(d+1)k_{ls}^2 - (k - v_B^2)]\lambda + h(k_{ls}^2) = 0,$$

where

$$\begin{aligned} h(k_{ls}^2) =& d k_{ls}^4 - [(d-1)F + dk - v_B^2] k_{ls}^2 \\ & + 2u_B v_B^3 - (F+k)(F+v_B^2). \end{aligned} \tag{20}$$

The necessary condition of system unstable is $h(k_{ls}^2) < 0$, for $k_{ls}^2 \in [0, 8]$.

4 Numerical simulation

In this section, a series of numerical simulations will be performed so that we can explore the dynamical behavior of the semi-discrete Gray-Scott model.

In all of the following simulations, the initial condition is always a small amplitude random perturbation 1 around the steady state. the size of the lattice is chosen to be 128×128, with periodic boundary conditions and the each of the 300000 times of iteration after v patterns .Secondly, the color selection of shaft as shown in figure 1 shows, the boundary of the right of a red, left, and the border blue for 0

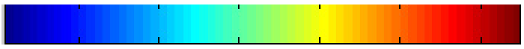
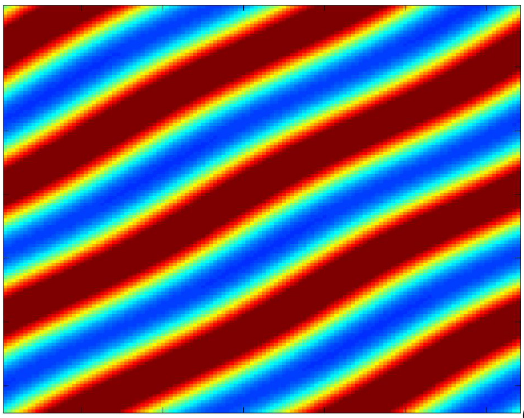
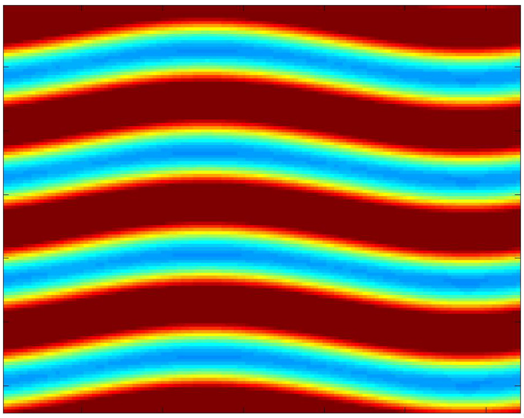


Figure 1: color shaft samples.



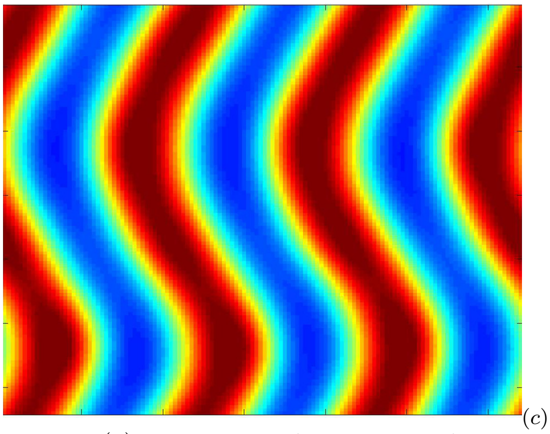
(a)

$(a) F = 0.0403, k = 0.0496, d = 10;$

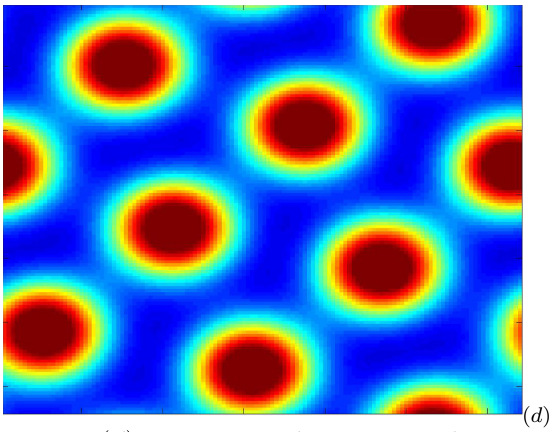


(b)

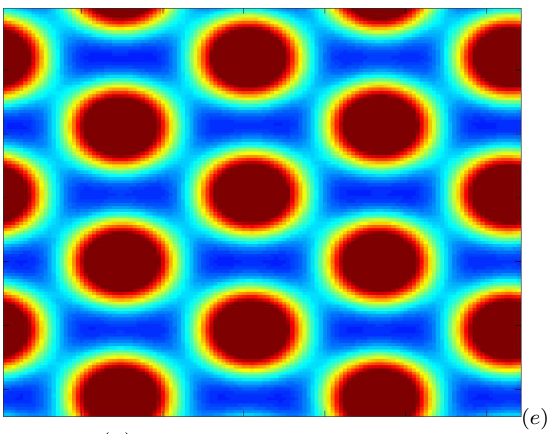
$(b) F = 0.0586, k = 0.0496, d = 10;$



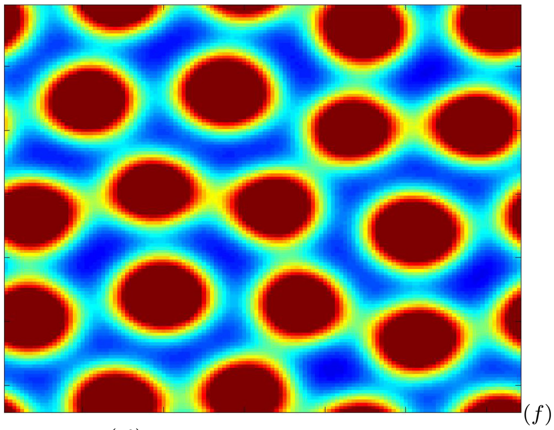
$(c) F = 0.0272, k = 0.0431, d = 10;$



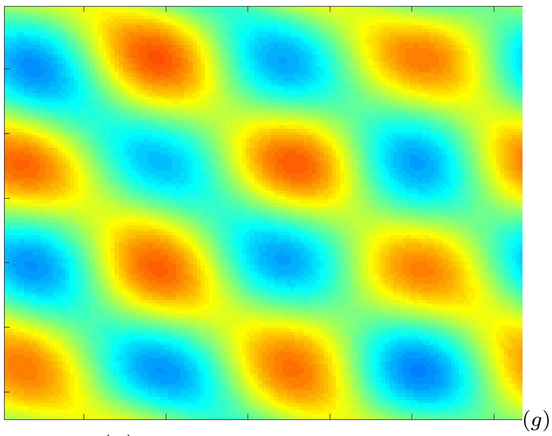
$(d) F = 0.0141, k = 0.0366, d = 11;$



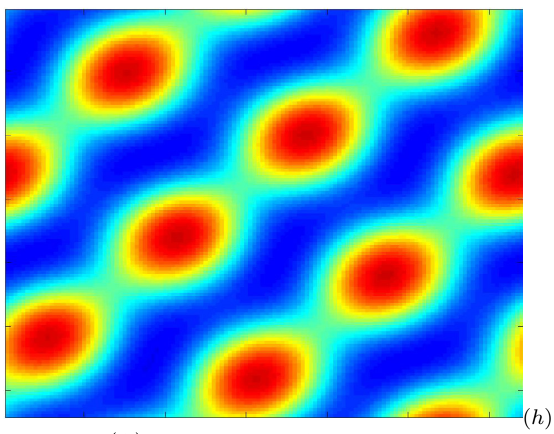
$(e) F = 0.0348, k = 0.0496, d = 10;$



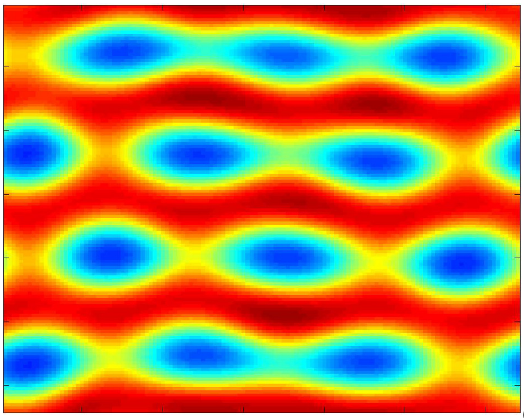
$(f) F = 0.0534, k = 0.056, d = 10;$



$(g) F = 0.0141, k = 0.0301, d = 10;$



$(h) F = 0.0141, k = 0.0366, d = 8;$

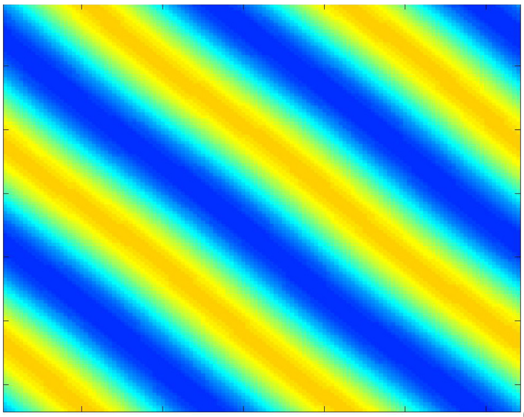

(i)

$(i) F = 0.0534, k = 0.056, d = 5.2.$

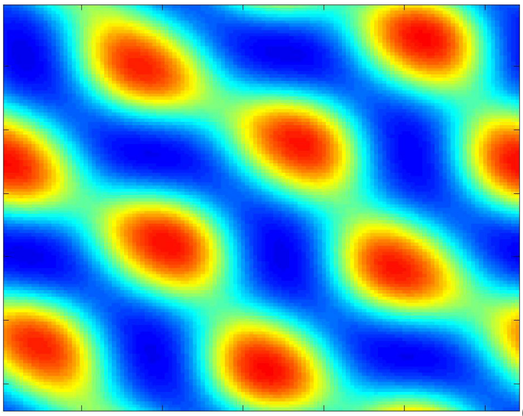
Figure 2: Striped, spotted and lace-liked Turing patterns of spatially discrete GS model(2).

Fig.2 shows all kinds of patterns with different parameter values which satisfy the conditions of Turing instability are obtained. Briefly, we only display several patterns of the substrate, v. The Turing patterns in first row are considered as striped patterns. Spotted and lace-liked Turing patterns are arraying on the second and third row respectively.

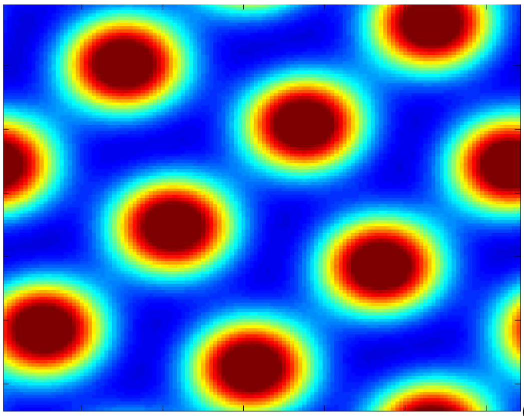
The G-S model (2) involves three parameters: d, k, F, in order to study the effects that parameters work on pattern formation, we assume that only one parameter is changing, others are remaining fixed, then Fig.2, Fig.3, Fig.4 are obtained.


(a)

$(a) F = 0.0141, k = 0.0366, d = 6;$

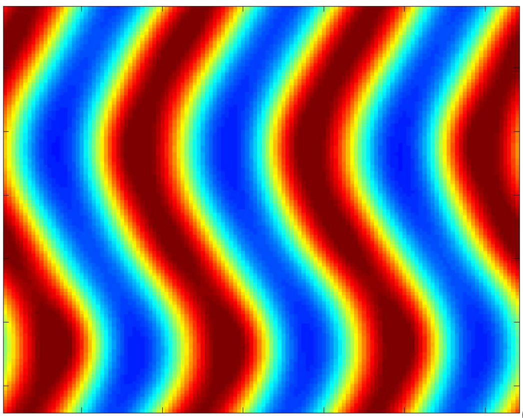

(b)

$(b) F = 0.0141, k = 0.0366, d = 7.5;$

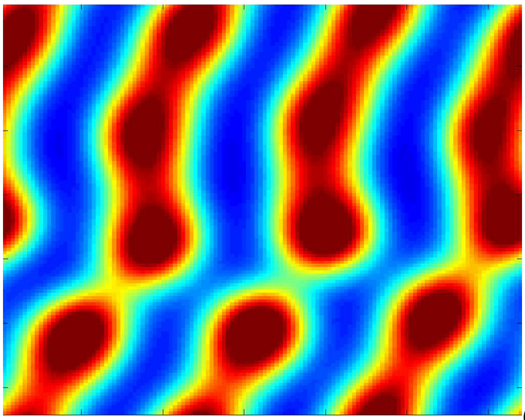

(c)

$(c) F = 0.0141, k = 0.0366, d = 11;$

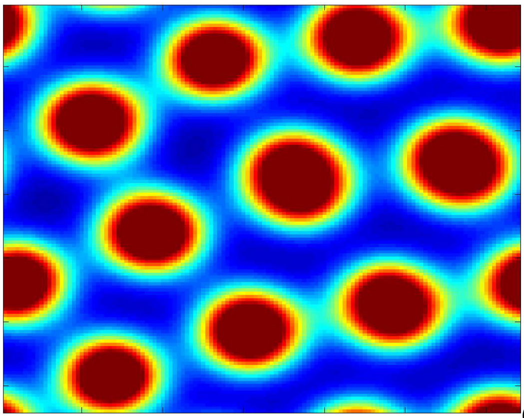
Figure 3: Turing patterns of spatially discrete GS model (2)


(a)

$(a) F = 0.0272, d = 10, k = 0.0431;$

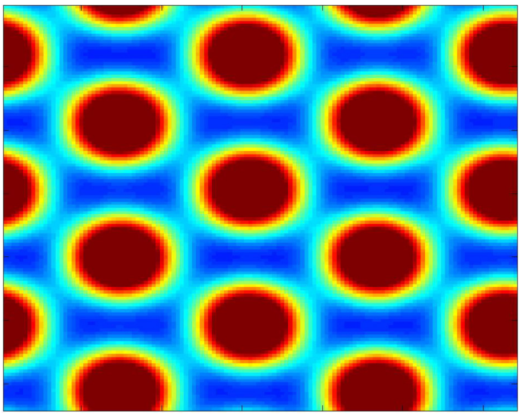


$(b)F = 0.0272, d = 10, k = 0.0452;$

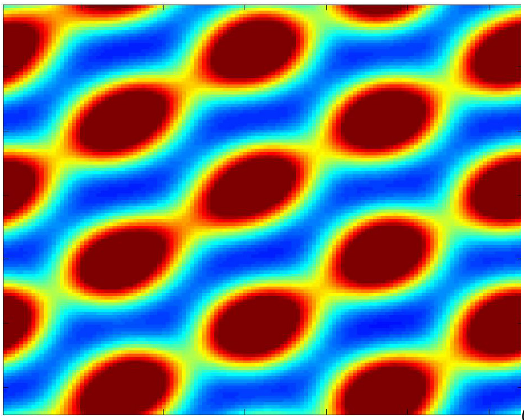


$(c)F = 0.0272, d = 10.k = 0.0511.$

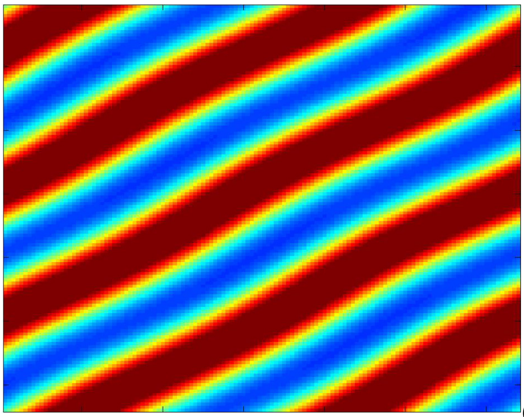
Figure 4: Turing patterns of spatially discrete GS model(2).



$(a)k = 0.0496, d = 10, F = 0.0348$



$(b)k = 0.0496, d = 10, F = 0.0372$



$(c)k = 0.0496, d = 10, F = 0.0403$

Figure 5: Turing patterns of spatially discrete GS model (2).

Firstly, in Fig.3, we choose parameters $F = 0.0141, k = 0.036$, d are chosen from the following set: $d = 6, 7.5, 11$. Via comparing the pattern structure, the transition from a striped to a spotted Turing pattern is received. Primitively, the system approaches a nearly stationary state with domains of clear stripes. With the gradually increase of d, lace-liked Turing pattern is found. Finally, isolated spots distribute in the whole space.

Secondly, we choose parameters $F = 0.0272, d = 10$. In fact, there exists only three main orientations for the arrangement of the pattern. Examples for these three configurations are shown in Fig.4. A phenomenon that stripes transit to spots is found. When k is relatively smaller, there are regular stripes in the space. With an increasing of k, a mixed Turing pattern that stripes break up, presenting a coexistence of spots and stripes, illustrated in Fig.(b). In Fig.(c), when k increases to 0.0511, stripes are no longer observed, substituted by a kind of absolutely isolated, anomalous spots.

Finally, in Fig.5, we fix $k = 0.0496, d = 10$. Different from Figure 3, 4, the transition from spots to stripes can be seen. When $F = 0.0348$, the space is full of orderly spots, see Fig.(a). As the increase of F, for example, $F = 0.0372$, see Fig.(b), specialty spots begin to connect, which comporting the near spots produce connecting by degrees and a tendency from orderly spots to regular stripes is observed. Continue to increasing F to 0.0403, see Fig.(c), clear and regular stripes are exposed.

5 Conclusions

In summary, in this paper, we have presented a theoretical analysis of Turing instability for a general semi-discrete system with the periodic boundary condition and the conditions of Turing instability for a semi-discrete G-S system follows immediately which describes a general two-variable kinetic model that represents an activator-substrate scheme.

Secondly , a large variety of new Turing pattern are obtained by number simulation in Turing instability region of semi-discrete G-S model. These Turing patterns are different from the patterns in the paper by Pearson [7], and we study that the dynamical behavior of this system depends on the parameters assuming that only one parameters changing, others are remaining fixed. When d (or k) varies and other parameters hold fixed, the pattern structure are changing from stripes to spots. In the contrast, when F varies and d, k are fixed, the transition from spots to stripes is observed.

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