Chapter 1

Spatio-temporal dynamics in a Turing model

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In this paper we study numerically two-dimensional spatio-temporal pattern formation in a generic Turing model, by investigating the dynamical behavior of a monostable system in the presence of Turing-Hopf bifurcation. In addition, we study the interaction of instabilities in a tristable system. We speculate that the interaction of spatial and temporal instabilities in Turing systems might bring some insight to a recent biological finding of temporal patterns on animal skin.

1.1 Introduction

In 1952 Alan Turing showed mathematically that a system of coupled reaction-diffusion equations could give rise to spatial concentration patterns of a fixed characteristic length from an arbitrary initial configuration due to diffusion-driven instability [1]. A remarkable feature of Turing systems as compared to other instabilities in systems out of equilibrium [2, 3] is that the characteristics of the resulting patterns are not determined by externally imposed length scales or constraints, but by the chemical reaction and diffusion rates intrinsic to the system.

Turing's goal was to model mechanisms behind morphogenesis, i.e., biological growth of form. Although genes play an important role in determining the anatomical structure of the resulting organism, from physical point of view they cannot explain spatial symmetry-breaking, which takes place as the cells start to differentiate. Turing hypothesized that as soon as the spherical blastula becomes large enough and there are some random deviations from the perfect symmetry, that state becomes unstable and the system is driven to another state defined by spontaneous physico-chemical processes. It has been qualitative shown that Turing models can indeed imitate biological patterns [4, 5], but the question whether morphogenesis really is a Turing-like process still remains.

The first experimental observation of a Turing pattern in a chemical reactor was due to De Kepper's group, who observed a spotty pattern in a chlorite-iodide-malonic acid (CIMA) reaction [6]. Later the results were confirmed by Ouyang and Swinney, who observed both striped and spotty patterns in extended systems [7]. The experimental observation of Turing patterns renewed the interest in these complex systems and subsequently a lot of research has been carried out employing theoretical [8, 9], computational [10, 11, 12] and experimental approaches [13].

Although Turing instability results in spatially periodic patterns that are stationary in time, in general reaction-diffusion system can also exhibit a variety of spatio-temporal phenomena [14, 15]. Hopf instability results in spatially homogeneous temporal oscillations and its relation to Turing instability is of great interest. This is because both instabilities can be observed experimentally in the CIMA reaction by varying the concentration of the color indicator in the reactor [15, 16]. The interaction between these instabilities [17] may take place either through a co-dimension-two Turing-Hopf bifurcation, when the corresponding bifurcation parameter threshold values are equal [18, 19] or due to different competing bifurcations of multiple stationary states [15, 20]. Both the situations result in interesting spatio-temporal dynamics. In addition, Yang et al. have recently obtained a variety of both stationary and oscillating structures in the numerical simulations of a system with interacting modes [21, 22].

In this article we report a study of Turing pattern formation in a two-species reaction-diffusion model with one or more stationary states. Simultaneous instability of many states results in competition between bifurcating states and the system exhibits spatial, temporal and spatio-temporal pattern formation depending on the system parameters. We are especially interested in the coupling of Turing and Hopf bifurcations, which results in periodic spatial patterns and temporal oscillations. In the next section we introduce and briefly analyze the model that we have used. Then, we present and discuss the results of our numerical simulations, which is followed by conclusions.

1.2 Analysis of the model

In this paper we use the so called generic Turing model [23], where the the temporal and spatial variation of normalized concentrations is described by the following reaction-diffusion system [24]

$$\begin{aligned} u_t &= D\nabla^2 u + \nu(u + av - uv^2 - Cuv) \\ v_t &= \nabla^2 v + \nu(bv + hu + uv^2 + Cuv), \end{aligned} \tag{1.1}$$

where the morphogen concentrations have been normalized so that $u = U - U_c$ and $v = V - V_c$, which makes $(u_c, v_c) = (0, 0)$ the trivial stationary solution. The term C adjusts the relative strength of the quadratic and cubic nonlinearities favoring the formation of either linear (2D stripes, 3D lamellae) or radial (2D spots, 3D droplets) Turing structures [23, 25]. D is the ratio of diffusion coefficients, whereas the linear parameters a, b, h and ν adjust the presence and type of instability.

For $h \neq -1$ the system of Eq. (1.1) has two other stationary states in addition to $(0, 0)$. These states are given by $u_c^i = -v_c^i/K$ and $v_c^i = -C + (-1)^i \pm \sqrt{C^2 - 4(h - bK)}/2$ with $K = (1 + h)/(a + b)$ and $i = 1, 2$. One should notice that the values of these stationary states depend also on the nonlinear parameter C. The characteristic equation corresponding to Eq. (1.1) can be written in the form

$$\lambda^2 + \left[(1 + D)k^2 - f_u - g_v\right] \lambda + Dk^4 - k^2(f_u + Dg_v) + f_u g_v - f_v g_u = 0, \quad (1.2)$$

where the partial derivatives of the reaction kinetics are given by

$$\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} = \nu \begin{pmatrix} 1 - v_c^2 - Cv_c & -2u_c v_c + a - Cu_c \\ v_c^2 + h + Cv_c & b + 2u_c v_c + Cu_c \end{pmatrix}. \quad (1.3)$$

Here u_c and v_c define the stationary state, whose stability we are studying. The dispersion relation $\mathrm{Re}\{\lambda(k)\}$ can be solved from Eq. (1.2). The real and imaginary parts of the eigenvalues corresponding to the single stationary state $(0, 0)$ are shown in Figure 1.1 for two sets of parameters corresponding to a Turing bifurcation (k_c unstable) and a Hopf bifurcation in a monostable system. The parameters used in Fig. 1.1 were $D = 0.122$, $a = 2.513$, $h = -1$, $b = -1.005$ and $\nu = 0.199$ for the Turing instability around $(0, 0)$ with critical wave number $k_c = 0.85$ and the same except $b = -0.8$ for the Hopf instability. For more details of the linear stability and pattern selection in the generic Turing model we refer the reader elsewhere [24].

From Fig. 1.1 one can observe that a Turing bifurcation corresponds to the case, where there is some k_i such that $\mathrm{Re}\{\lambda(k_i)\} > 0$ and $\mathrm{Im}\{\lambda(k_i)\} = 0$. On the other hand, a Hopf bifurcation corresponds to the situation, where a pair of imaginary eigenvalues crosses the real axis, i.e., there is some k_i with $\mathrm{Re}\{\lambda(k_i)\} > 0$ and $\mathrm{Im}\{\lambda(k_i)\} \neq 0$. The parameters can also be adjusted such that $k_c = 0$ for Turing instability or so that there is a combined Turing-Hopf bifurcation from one stationary state. The condition for the Hopf bifurcation in the system of Eq. (1.1) is $b > -1$ and for the Turing bifurcation it is $b < (1 - \sqrt{-4Dah})/D$ [24]. If the parameter $h < -1$ the stationary state $(0, 0)$ goes through a subcritical pitchfork bifurcation [2]. For $h > -1$ a tristability is established, i.e., there are three stationary states.

1.3 Numerical simulations

We have performed extensive numerical simulations of the generic Turing model (Eq. (1.1)) in two-dimensional domains of size 100×100 by using parameter

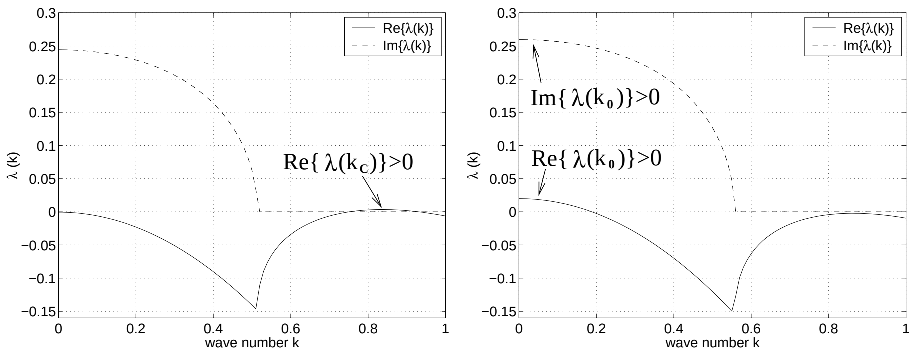

Figure 1.1: The largest eigenvalue of the linearized system corresponding to a Turing (left) and Hopf bifurcation (right). The real and imaginary parts of the eigenvalues correspond to solid and dashed lines, respectively.

values corresponding to different bifurcation and stability scenarios. The time integration of the discretized problem was carried out by using the Euler method ($dx = 1$ and $dt = 0.01$). On one hand, we have studied the interaction of Turing and Hopf bifurcations in a monostable system, and on the other hand, a tristable system with a coupled Turing-Hopf-Turing or Turing-Turing bifurcation. These conditions result in a variety of spatio-temporal dynamics, whose characterization is very challenging.

By using the parameters $D = 0.122$, $a = 2.513$, $h = -1$, $b = -.95$, $\nu = 0.199$ and $C = 1.57$ one can adjust the system in such a way that there is only one stationary state $(0, 0)$, which is both Turing unstable with $k_c = 0.85$ and characteristic length $L = 2\pi/k_c \approx 7.4$, and Hopf unstable with oscillation period of $T_c = 2\pi/\mathrm{Im}\{\lambda(k_0)\} \approx 25.40 = 2540 \times dt$ ($k_c = 0$). Eventually, the oscillations fade away and a stationary hexagonal spotty pattern is established. Fig. 1.2 shows snapshots of the behavior of the system at arbitrary moments of time. The homogeneous domains changing color correspond to oscillations.

By fixing $h = -0.97 \neq -1$ we admitted two additional stationary states and studied the pattern formation with parameters $D = 0.516$, $a = 1.112$, $b = -0.96$ and $\nu = 0.450$, which correspond to a Turing-Hopf bifurcation of the state $(0, 0)$ with $k_c = 0.46$ and Turing bifurcation of the stationary states $(-2.01, 0.40)$ and $(9.97, -1.97)$, both with $k_c = 0$. The Turing-Hopf modes growing from $(0, 0)$ excite the former of these two states, which results in a coupling between Turing-Hopf and Turing instabilities. From random initial configuration the parameter selection $C = 1.57$, which corresponds to spotty patterns [24] resulted in a hexagonal lattice with a few twinkling spots at dislocation sites. Twinkling hexagonal lattices of spots have previously been obtained in numerical simulations of a four-component Turing model [21] and of a nonlinear optical system [26]. Our results show that "twinkling-eye" behavior can also be observed in a two-component model without any special preparations [27].

Using the same parameters as above, except choosing $b = -1.01$ one still ob-

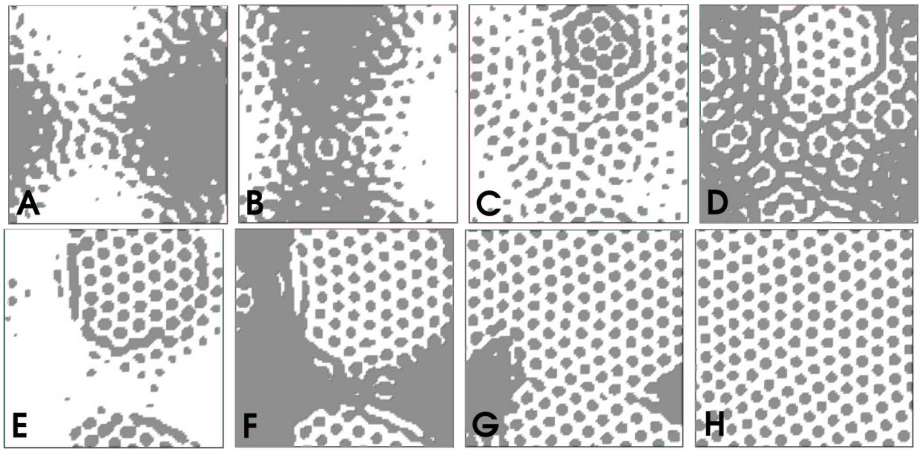

Figure 1.2: A two-dimensional concentration patterns obtained in a system with a coupled Turing-Hopf bifurcation as the simulation is started from a random initial configuration. White and gray domains correspond to areas dominated my chemical u and v, respectively. The time evolution goes from left to right and from top to bottom [27].

tains a tristable system, although the stationary state $(0,0)$ is no longer Turing-Hopf unstable, but Turing unstable with $k_c = 0.46$. The two other stationary states $(-1.191, 0.350)$ and $(6.529, -1.920)$ are Turing unstable with $k_c = 0$ as in the previous case. Again the Turing modes growing from $(0,0)$ excite another nearest stationary state, which results in an interesting competition between growing modes. Although there is no straightforward Turing-Hopf bifurcation, the modes growing from the state $(-1.191, 0.350)$ with $Re\{\lambda(k_0)\} > 0$ are coupled with the damped Hopf modes $\propto e^{i\omega_0 t}$ of the state $(0,0)$, which results in oscillatory behavior with period $T_c \approx 3765 \times dt$. This dynamics is described by a series of snapshots in Fig. 1.3, where the homogeneous oscillations sweep out spots with period T_c, and then the spots are again nucleated at the centers of concentric target pattern waves. The competition continues for long times of up to $10^6 \times dt$, although the oscillations gradually fade out.

One should mention that for parameter value $C = 0$, which has been shown to correspond to a striped pattern [24], the system showed a straightforward Turing bifurcation of the state $(0,0)$ without any oscillatory competition. This happened because the Turing modes growing from the state $(0,0)$ and resulting in stripes did not excite the other stationary states, i.e., the amplitude of the striped concentration pattern was not large enough for the modes to interact with other stationary states. Based on this observation, one can state that in multistable systems the parameter selection might have drastic effects on the dynamical behavior of the system.

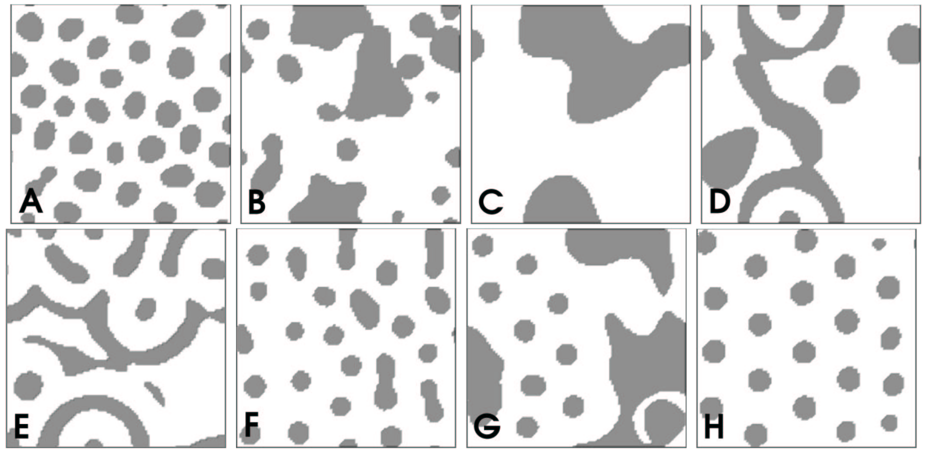

Figure 1.3: The two-dimensional concentration patterns obtained in a tristable system with a coupled Turing-Hopf-Turing bifurcation as the simulation is started from a random initial configuration. The time evolution goes from left to right and from top to bottom [27].

1.4 Conclusions

In this paper we have studied spatio-temporal pattern formation in the generic Turing model. Most of the studies of spatio-temporal dynamics have in general been carried out in one-dimensional systems, since they make it feasible to study the Turing-Hopf interaction by using amplitude equation formalism [15, 18]. In the two-dimensional case (not to talk about three dimensions) the studies of spatio-temporal behavior have typically, although not always [28], been more or less qualitative. By considering stability and bifurcation aspects one can govern and interpret the behavior of the systems to some extent, but otherwise two-dimensional spatio-temporal dynamics is often too complex to be studied analytically.

By using different parameter sets we have studied the Turing-Hopf coupling in a monostable system, which resulted transient oscillatory behavior combined with localized spotty and oscillatory domains. By establishing a tristability in a similar system we obtained a hexagonally arranged spotty pattern with a few twinkling spots, i.e., spots appearing and disappearing at dislocation sites. The tristability without straightforward Turing-Hopf bifurcation resulted in temporal competition since the stable Hopf modes of one stationary state were coupled with the Turing bifurcation of another state, caused by competition between a homogeneous oscillatory wave and a spotty pattern. In addition, we have observed that different parameter values might prevent this coupling and instead pure stationary Turing stripes would settle in.

Turing instability is not relevant only in reaction-diffusion systems, but also in describing other dissipative structures, which can be understood in terms of diffusion-driven instability. Turing instability has been discussed in relation to gas discharge systems [29], catalytic surface reactions [30], semiconductor nanostructures [31], and surface waves on liquids [32]. The studies of temporal and spatial pattern formation in Turing system are important, since they may be of great interest also in biological context, e.g. skin hair follicle formation, which is closely related to skin pigmentation, occurs in cycles [33]. Recently, spatio-temporal traveling wave pattern has been observed on the skin of a mutant mouse [34], which might perhaps be the result of a misconfigured Turing mechanism with competing instabilities, i.e., the pattern becomes temporal instead of stationary due to a shift in the values of the reaction and diffusion rates of morphogens.

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