

THE EFFECT OF DIFFUSION ON MULTISTABILITY AND STOCHASTIC SENSITIVITY IN SPATIALLY EXTENDED SYSTEMS

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Article history:

Received 12.05.2024, Accepted 16.09.2024

Abstract

A spatially-extended reaction-diffusion model is considered. The work is focused on self-organization mechanisms of diffusion instability and Turing pattern formation. Pattern generation and multistability of the system is demonstrated for varying diffusion intensity. In the stochastic variant of the model, the sensitivity of coexisting patterns to noise is studied. The stochastic sensitivity function technique is used for the analysis of noise-induced transitions between patterns. Application of stochastic sensitivity functions is discussed on examples.

Key words

Nonlinear systems, self-organization, Turing patterns, stochastic sensitivity

1 Introduction

One of the most vital fields of research in modern science is the study of self-organization dynamics in complex non-linear systems [Nicolis and Prigogine, 1977], [Cross and Greenside, 2009]. Such systems and phenomena of spontaneous ordering are often encountered in theoretical and applied natural sciences [Deichmann, 2023], [Martinez et al., 2022], [Odagaki, 2021]. The apparatus of mathematical modeling and computer simulations is a valuable approach used in analysis of nonlinear dynamics in these systems [Kazarnikov et al., 2023]. In some systems computer modeling methods are usually preferred over the real experiment, especially when experimentation is too complex or expensive.

In reaction-diffusion systems the phenomenon of Turing instability and pattern formation can be considered an example of self-organization mechanism [Turing, 1952]. Systems with strong diffusion form a sta-

ble spatially homogeneous equilibrium state. Turing's work describes conditions when this equilibrium becomes unstable and a non-homogeneous wave-like state (a Turing pattern) is preferred by the system [Kavallaris et al., 2023]. Usually several patterns with varying spatial frequency coexist in the same parametric domain. Such multistability is evident when the initial state of the system is varied for fixed set of system parameters [Kolinichenko and Ryashko, 2020], [Liu et al., 2022].

Noise-induced effects play a crucial role in systems with self-organization [Hausenblas et al., 2020], [Aguirre and Kowalczyk, 2022], [Alexandrov et al., 2021]. Random perturbations greatly affect system dynamics and produce stochastic phenomena, that could not be observed when the effect of noise is excluded. An important field of work in this study is to research and provide efficient methods that allow measurement of noise effects and prediction of system behavior. One such example involves stochastic sensitivity functions (SSF) [Bashkirtseva et al., 2013], [Bashkirtseva et al., 2020], [Bashkirtseva and Ryashko, 2021]. This technique is useful for investigation of probabilistic distributions around attractors and limit cycles. It is helpful for building confidence intervals of random states in continuous and discrete nonlinear systems.

Recent work on stochastic phenomena in spatially extended reaction-diffusion systems involves investigation of noise-induced pattern transitions [Horsthemke and Lefever, 1984], [Bashkirtseva et al., 2021], [Muntari and Şengül, 2022]. This includes parametric analysis of stochastic sensitivity and transition probability between coexisting patterns–attractors. It is shown, that variation of parameters that regulate system dynamics, especially diffusion intensity ratio, affect pattern preference dynamics.

In this work, the spatially-extended stochastic reaction-diffusion model is studied. It is shown, that in the parametric domain of Turing instability the system forms non-homogeneous patterns. Multistability of the system and the effect of diffusion variation on the diversity of coexisting patterns is studied.

The main focus of the paper is the phenomenon of noise-induced transitions between coexisting patterns. Relation between such transitions and stochastic sensitivity of patterns–attractors is discussed. Probabilistic distributions of noisy states near patterns are described by statistical data from direct computer modeling. The analytical stochastic sensitivity functions technique (SSF) [Kolinichenko et al., 2023] is applied for description of these distributions. With the SSF technique the influence of varying diffusion intensity on pattern preference mechanisms is discussed on examples.

2 Model introduction

Consider the following stochastic variant of the spatially-extended Brusselator model [Prigogine and Lefever, 1968]:

$$\begin{aligned} \frac{\partial u}{\partial t} &= a - (b+1)u + u^2v + D_u \frac{\partial^2 u}{\partial x^2} + \varepsilon \xi(t, x) \\ \frac{\partial v}{\partial t} &= bu - u^2v + D_v \frac{\partial^2 v}{\partial x^2} + \varepsilon \eta(t, x). \end{aligned} \quad (1)$$

Here, the system variable functions $u(t, x)$ and $v(t, x)$ are the dimensionless concentrations of reagents. Positive parameters a and b define the reaction process dynamics, D_u and D_v are the intensity of diffusion of the respective reagents. The additive random noise is represented by two stochastic components $\xi(t, x)$ and $\eta(t, x)$ - two uncorrelated white Gaussian noises, the coefficient ε is the additive noise intensity.

The spatial variable x varies within a bounded spatial domain, which is the unit segment $[0, 1]$. Boundary conditions are the zero-flux conditions:

$$\begin{aligned} \frac{\partial u}{\partial x}(0, 0) &= \frac{\partial u}{\partial x}(0, 1) = 0 \\ \frac{\partial v}{\partial x}(0, 0) &= \frac{\partial v}{\partial x}(0, 1) = 0. \end{aligned} \quad (2)$$

Without diffusion components ($D_u = D_v = 0$) and random noise ($\varepsilon = 0$) the system has an equilibrium $(\bar{u}, \bar{v}) = (a, \frac{b}{a})$, which is stable if $b < (a+1)^2$.

For a deterministic ($\varepsilon = 0$) system (1), (2) with diffusion, one may consider the spatially homogeneous equilibrium state $u(t, x) = \bar{u}$, $v(t, x) = \bar{v}$. A special case of instability of such state is the diffusion instability or Turing instability. It occurs if the equilibrium of the model without diffusion is stable and the following Turing instability condition is met:

$$\frac{D_u}{D_v} < \left(\frac{\sqrt{b} - 1}{a} \right)^2. \quad (3)$$

Such instability causes formation Turing patterns - stable spatially non-homogeneous wave-like structures. In this article consider the parameter values $a = 3$, $b = 9$ fixed as in [Kolinichenko and Ryashko, 2020]. The equilibrium values are $\bar{u} = 3$, $\bar{v} = 3$. The condition (3) is met if diffusion coefficient ratio is $\frac{D_u}{D_v} < \frac{4}{9}$, therefore the spatially homogeneous equilibrium becomes unstable and pattern formation is expected. Figure 1 demonstrates pattern formation process from a randomly generated state for $D_u = 0.016$, $D_v = 0.1$. For simplicity only the $u(t, x)$ component of system state is shown, the $v(t, x)$ has similar structure.

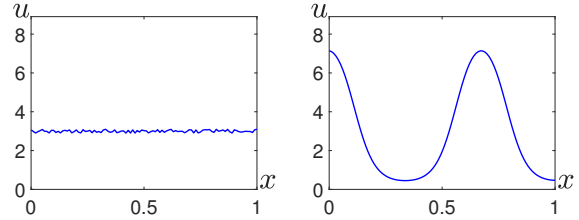


Figure 1. Turing pattern formation for system (1), (2) with parameters $a = 3$, $b = 9$, $D_u = 0.016$, $D_v = 0.1$: $u(x)$ of random initial state (left) and of pattern (right)

The spatiotemporal evolution of the system can be demonstrated as a color diagram in Figure 2. Here, the spatial variable varies along the vertical axis, time varies along the horizontal axis and color represents the value of $u(t, x)$. It is evident, that the random state quickly evolves into a definite stable pattern.

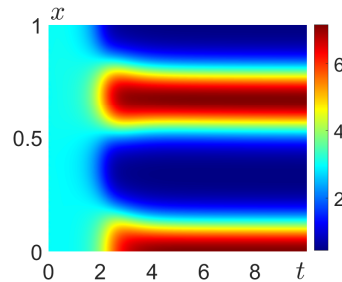


Figure 2. Turing pattern formation for system (1), (2) with parameters $a = 3$, $b = 9$, $D_u = 0.016$, $D_v = 0.1$: spatiotemporal evolution of $u(t, x)$

Each pattern can be assigned a symbol, based on the spatial frequency or the number of wavelengths within the spatial domain and the tendency of the u component near the domain's left edge ($x = 0$). Note, that

Table 1. Multistability in the spatially-extended Brusselator

k	$D_u = 0.002$	$D_u = 0.016$	$D_u = 0.032$
0.5	4.5 ↓, 4.5 ↑	2 ↑, 2 ↑	1 ↑, 1 ↑
1	4 ↑, 4 ↑	2 ↑, 2 ↑	1 ↑, 1 ↓
1.5	3 ↑, 3 ↑	1.5 ↑, 1.5 ↓	1.5 ↑, 1.5 ↓
2	4 ↑, 4 ↑	2 ↑, 2 ↓	1 ↑, 1 ↓
2.5	5 ↑, 5 ↑	1.5 ↑, 1.5 ↓	1.5 ↑, 1.5 ↓
3	5 ↑, 4 ↑	2 ↑, 2 ↓	1 ↑, 1 ↓
3.5	3.5 ↑, 3.5 ↓	1.5 ↑, 1.5 ↓	1.5 ↑, 1.5 ↓
4	4 ↑, 4 ↓	2 ↑, 2 ↓	1 ↑, 1 ↓
4.5	4.5 ↑, 4.5 ↓	1.5 ↑, 1.5 ↓	1.5 ↑, 1.5 ↓
5	5 ↑, 5 ↓	2 ↑, 2 ↓	1 ↑, 1 ↓
Total	9	4	4

due to the boundary conditions (2) being the Neumann conditions, the number of wavelengths is either integer or half-integer. The pattern demonstrated in Figures 1 and 2 can be assigned the symbol 1.5 ↓: a full wave and half a wave fit in the spatial domain and the concentration curve u declines near $x = 0$.

Frequently, such systems display multistability: depending on the initial condition, the system can generate several patterns— attractors that coexist within the same parametric domain. Figure 3 shows an example of coexisting 1.5 ↑ and 2 ↓ patterns.

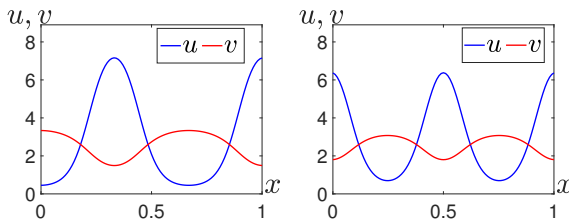


Figure 3. System (1), (2) with $a = 3, b = 9, D_u = 0.016, D_v = 0.1$: coexisting 1.5 ↑ pattern (left) and 2 ↓ pattern (right)

A degree of multistability can be measured by the amount of different coexisting patterns. While in some cases only few patterns are seen, in others the number of patterns can be large. One of the main points of interest in the study of multistability is to investigate the effect of system parameter variation on the number of coexisting states. Knowing that the pattern structure is wave-like and considering the boundary conditions (2), the following form of initial state variation is used:

$$\begin{aligned} u(0, x) &= \bar{u} + j\gamma \cos(2k\pi x), \\ v(0, x) &= \bar{v} - j\gamma \cos(2k\pi x). \end{aligned} \tag{4}$$

Here (\bar{u}, \bar{v}) is the equilibrium of system (1) with $D_u = D_v = 0$. The parameter k is the wave number of the cosine wave, which can be integer or half-integer due to the boundary conditions (2). The parameter j is either 1 or -1 and is responsible for the tendency of the spatial wave on the left edge of the spatial domain. In our simulations the amplitude of the wave is $\gamma = 0.1$. Using different initial states generated by form (4) various distinct patterns were obtained.

This experiment with multistability is performed for three pairs of diffusion coefficients: (i) $D_u = 0.002, D_u = 0.0125$, (ii) $D_u = 0.016, D_v = 0.1$, (iii) $D_u = 0.032, D_u = 0.2$. In all cases the diffusion coefficient ratio is $\frac{D_u}{D_v} = 0.16$. The results are shown in Table 1, where each cell contains two pattern symbols: left for $j = -1$ and right for $j = 1$.

The results in this series of simulations imply that for greater diffusion coefficients there are fewer coexisting patterns. This is demonstrated by the nine different patterns encountered for $D_u = 0.002$ and four different patterns for $D_u = 0.016$ and $D_u = 0.032$. The spatial frequency of coexisting patterns decreases: for $D_u = 0.002$ the spatial domain contains up to five wavelengths, while the maximum number of wavelengths is two for $D_u = 0.016$ and one and a half for $D_u = 0.032$.

When diffusion coefficients were increased to certain larger values, patterns were no longer observed. For example, for $D_u = 0.68, D_v = 4.25$ pattern formation does not occur even though condition (3) is satisfied. At this point the patterns with the smallest possible spatial frequency, the 0.5 ↑ and 0.5 ↓ are not generated and the homogeneous equilibrium is observed.

3 Stochastic sensitivity analysis

Consider the system (1), (2) with $\varepsilon > 0$ when spatiotemporal dynamics are affected by random noise. It is implied that different patterns respond differently to such effects. While some patterns remain mostly unaffected, others can deteriorate. A special case of stochastic process is the stochastic transition between coexisting patterns— attractors. It is assumed, that a sensitive pattern disperses under the effect of noise and instead the system will generate a less sensitive pattern. To demonstrate such process, let $a = 3, b = 9, D_u = 0.016, D_v = 0.1$ and the initial state is the 2 ↓ pattern (see Figure 3). Modeling process is initiated with noise intensity $\varepsilon = 0.5$. During the simulations the pattern is transformed into a noisy 1.5 ↓ pattern. The initial and the final states of this simulation are shown in Figure 4.

Temporal details of modeling process are displayed on Figure 5. Here, the process of the 2 ↓ pattern destruction is evident. The 1.5 ↓ pattern remains relatively unchanged for the remainder of the simulation. The transition itself appears to be sharp and irreversible, which

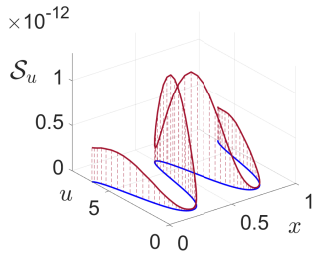


Figure 6. Mean-square deviation \mathcal{S}_u of $u^\varepsilon(t, x)$ from $2 \downarrow$ pattern in system (1), (2) for $a = 3, b = 9, D_u = 0.016, D_v = 0.1, \varepsilon = 10^{-6}$

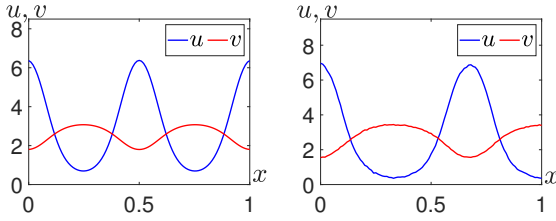


Figure 4. Noise-induced transition from $2 \downarrow$ to $1.5 \downarrow$ for system (1), (2) with $a = 3, b = 9, D_u = 0.016, D_v = 0.1, \varepsilon = 0.5$: initial (left) and final (right) states

implies that the $2 \downarrow$ pattern is more sensitive to noise. If the same experiment is performed with the $1.5 \downarrow$ pattern as the initial condition of the system (1), (2), the transition to a different pattern does not occur. It is assumed,

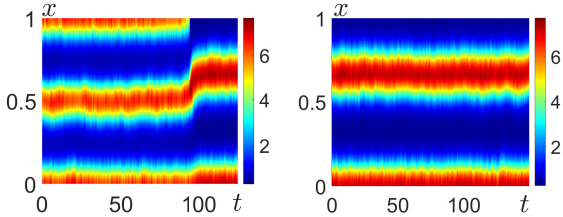


Figure 5. Stochastic spatiotemporal evolution of $u(t, x)$ in system (1), (2) for $a = 3, b = 9, D_u = 0.016, D_v = 0.1, \varepsilon = 0.5$: transition from $2 \downarrow$ to $1.5 \downarrow$ transition (left), no transition from $1.5 \downarrow$ (right)

that the system state can deviate too far from a pattern-attractor under the effect of random noise. In this case the system state tends toward an attractor, which is more resistant to noise.

In order to compare the noise sensitivity of coexisting patterns quantitatively, the following statistical approach is suggested. The noise intensity ε is set to a low value in order to avoid a pattern destruction. The initial state of the stochastic system (1), (2) is a specific pattern. A

series of numerical simulations is performed and mean-square deviation (5) is evaluated:

$$\begin{aligned} \mathcal{S}_u(x, \varepsilon) &= E(u^\varepsilon(t, x) - u^*(x))^2, \\ \mathcal{S}_v(x, \varepsilon) &= E(v^\varepsilon(t, x) - v^*(x))^2. \end{aligned} \quad (5)$$

Here, $u^*(x)$ and $v^*(x)$ are components of the considered deterministic pattern. The $u^\varepsilon(t, x)$ and $v^\varepsilon(t, x)$ are the stochastic states obtained from simulations with noise intensity $\varepsilon > 0$.

Figure 6 shows the example results of this approach for u component of the $2 \downarrow$ pattern. Mean-square deviation of random states near the pattern is a non-homogeneous function. Maximums of this function localize parts of the pattern most sensitive to noise.

It is possible to compare mean-square deviation of different patterns. Figure 7 shows results of such comparison. It is shown, that generally the mean-square deviation of $2 \downarrow$ pattern is greater than that of $1.5 \downarrow$. This result aligns with the transition dynamics and preference shown in Figure 5.

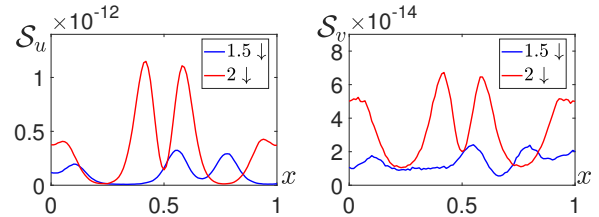


Figure 7. Mean-square deviation of $2 \downarrow$ (red) and $1.5 \downarrow$ (blue) patterns in system (1), (2) for $a = 3, b = 9, D_u = 0.016, D_v = 0.1, \varepsilon = 10^{-6}$

While this approach provides useful information on stochastic sensitivity, it requires large amounts of numerical simulations and computational time for accurate statistical data. An analytical approach based on the stochastic sensitivity function technique used in ordinary differential equation systems analysis can be applied for approximation of mean-square deviation (5).

Consider a discretized spatial domain $[0, 1]$: x_0, x_1, \dots, x_{n+1} where $x_i = ih, h = 1/(n+1)$. The pattern components $u^*(x), v^*(x)$ are represented by their approximation on the spatial grid: $u_i^* = u^*(x_i)$ and $v_i^* = v^*(x_i)$. Discretized derivatives of functions $f(u, v) = a - (b+1)u + u^2v$ and $g(u, v) = bu - u^2v$ are defined as follows:

$$\begin{aligned} a_i &= \frac{\partial f}{\partial u}(u_i^*, v_i^*), & b_i &= \frac{\partial f}{\partial v}(u_i^*, v_i^*) \\ q_i &= \frac{\partial g}{\partial u}(u_i^*, v_i^*), & m_i &= \frac{\partial g}{\partial v}(u_i^*, v_i^*). \end{aligned}$$

Denote $\alpha = \frac{D_u}{h^2}$ and $\beta = \frac{D_v}{h^2}$. Then consider the matri-

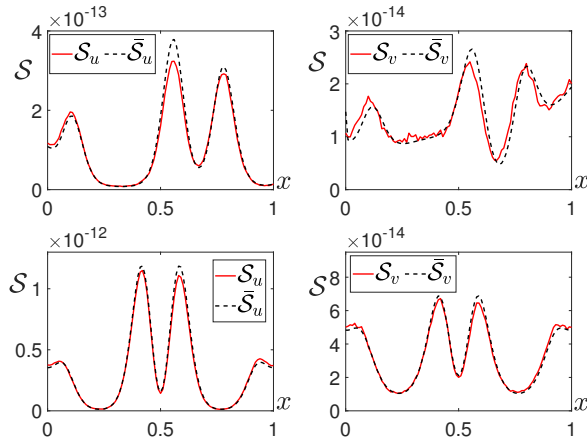


Figure 8. Mean-square deviation found by direct simulations (red) and SSF estimation (dashed) in system (1), (2) for $a = 3$, $b = 9$, $D_u = 0.016$, $D_v = 0.1$, $\varepsilon = 10^{-6}$ for $1.5 \downarrow$ pattern (up) and $2 \downarrow$ pattern (down)

ces

$$A = \begin{bmatrix} a_1 - \alpha & \alpha & 0 & \dots & 0 \\ \alpha & a_2 - 2\alpha & \alpha & \dots & 0 \\ 0 & \alpha & a_3 - 2\alpha & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & a_n - \alpha \end{bmatrix},$$

$$M = \begin{bmatrix} m_1 - \beta & \beta & 0 & \dots & 0 \\ \beta & m_2 - 2\beta & \beta & \dots & 0 \\ 0 & \beta & m_3 - 2\beta & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & m_n - \beta \end{bmatrix}.$$

$$B = \text{diag}[b_1, \dots, b_n], \quad Q = \text{diag}[q_1, \dots, q_n],$$

$$F = \begin{bmatrix} A & B \\ Q & M \end{bmatrix},$$

For considered discretization, the stochastic sensitivity matrix W of the pattern $(\bar{u}(x), \bar{v}(x))$ is a solution of the matrix equation (6):

$$FW + WF^\top + S = 0. \quad (6)$$

Here, S for system (1), (2) is a unit $2n \times 2n$ -matrix. The stochastic sensitivity functions for the pattern-attractor are defined by the matrix W as follows:

$$\begin{aligned} \mathcal{W}_u(x_i) &= W_{i,i}, \quad i = 1, 2, \dots, n \\ \mathcal{W}_v(x_i) &= W_{i,i}, \quad i = n + 1, n + 2, \dots, 2n. \end{aligned} \quad (7)$$

This function and the mean-square deviation (5) are related as shown in (8):

$$\begin{aligned} \mathcal{S}_u(x, \varepsilon) &\approx \bar{\mathcal{S}}_u(x, \varepsilon) = \varepsilon^2 \mathcal{W}_u(x), \\ \mathcal{S}_v(x, \varepsilon) &\approx \bar{\mathcal{S}}_v(x, \varepsilon) = \varepsilon^2 \mathcal{W}_v(x). \end{aligned} \quad (8)$$

The approximation of random state distribution for different patterns, including the results shown in Figure 7, is demonstrated in Figure 8. It aligns well with statistical data and can be obtained relatively fast as it requires to solve only the system (6). Modern software packages for linear algebra are able to check the equation for solution existence and quickly find it.

The influence of system parameter variation on pattern preference can be studied through analysis of stochastic sensitivity. For parametric analysis of stochastic sensitivity it is useful to have a numeric characteristic. For example, consider the maximum sensitivity values (9):

$$\begin{aligned} \bar{\mathcal{W}}_u &= \max_{x \in [0,1]} \mathcal{W}_u(x), \\ \bar{\mathcal{W}}_v &= \max_{x \in [0,1]} \mathcal{W}_v(x). \end{aligned} \quad (9)$$

With these numeric characteristics in mind, parametric analysis of system (1), (2) is performed with varying diffusion intensity. The diffusion coefficient ratio remains constant $\frac{D_u}{D_v} = 0.16$. For simplicity, the horizontal axis displays only the D_u parameter variation, however D_v is also varied so that the ratio will remain the same. The results are shown in Figure 9.

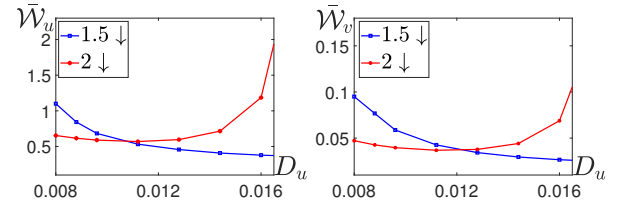


Figure 9. Stochastic sensitivity of coexisting patterns in system (1), (2) for $a = 3$, $b = 9$ and $\frac{D_u}{D_v} = 0.16$: Maximum sensitivity values $\bar{\mathcal{W}}_u$ (left) and $\bar{\mathcal{W}}_v$ (right) for varying diffusion

The first evident result is that the $2 \downarrow$ pattern becomes less sensitive for lower diffusion coefficients. It is expected that the pattern will remain mostly unaffected by random noise in contrast to the results shown in Figure 5 and transition to another pattern will not occur. Another interesting result is that the $1.5 \downarrow$ pattern becomes more sensitive for lower diffusion coefficients. The $2 \downarrow$ pattern appeared more sensitive than $1.5 \downarrow$ for $D_u = 0.016$, $D_v = 0.1$ and had higher chance of transition, while for $D_u = 0.0088$, $D_v = 0.055$ the situation is opposite. Figure 9 shows that for $D_u = 0.0088$, $D_v = 0.055$ the $1.5 \downarrow$ pattern is more sensitive than $2 \downarrow$ pattern. It is now expected that destruction of the $1.5 \downarrow$ pattern is more probable. Figure 10 shows an example of spatiotemporal dynamics for these diffusion coefficients.

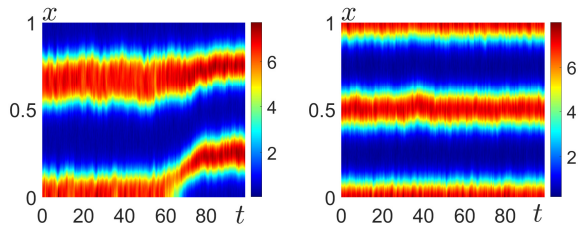


Figure 10. Stochastic spatiotemporal evolution of $u(t, x)$ in system (1), (2) for $a = 3$, $b = 9$, $D_u = 0.0088$, $D_v = 0.055$, $\varepsilon = 0.7$: transition from 1.5 \downarrow to 2 \uparrow (left), no transition from 2 \downarrow (right)

It should be emphasized, that the ratio of diffusion coefficients is the key variable which defines the Turing instability condition directly and controls deterministic pattern formation. Here, it is shown that even if the ratio is constant, the variation of D_u and D_v affects spatiotemporal and stochastic dynamics significantly.

4 Conclusion

In this paper, the stochastic spatially-extended Brusselator model (1), (2) was studied. Multistability of system without noise was demonstrated and studied for varying values of diffusion coefficients. Increasing diffusion intensity leads to less number of coexisting Turing patterns in the same set of parameters. It is emphasized, that when diffusion intensity of the activator and the inhibitor of the system is varied proportionally, the number of patterns changes, even if the ratio is constant and satisfies the Turing instability condition (3). It is implied that significant proportional increase of diffusion intensity can suppress pattern formation. The phenomenon of stochastically forced transitions between coexisting patterns was demonstrated on examples. Random noise causes destruction of a sensitive pattern with subsequent generation of noise resistant pattern. Two approaches to stochastic sensitivity measurement are discussed. Mean-square deviation of random states around pattern can be estimated with the application of stochastic sensitivity functions technique. With this approach the effect of diffusion intensity variation on stochastic sensitivity and pattern preference was investigated.

Acknowledgements

The work has been supported by Ministry of Science and Higher Education of the Russian Federation “Ural Mathematical Center” (N 075-02-2024-1428).

The elaboration of the stochastic sensitivity theory of the patterns–attractors and application of this theory to models forced by random disturbances was supported by Russian Science Foundation (N 24-11-00097).

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