Singularities and chaos in coupled systems*

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Abstract

In [7] we proved that a system consisting of two brusselators linearly coupled by diffusion contains strange attractors. In this paper we will give numerical examples of the chaotic behaviour predicted by the theoretical results. Some details about error analysis, not included in [7], will be supplied here.

1 Introduction

Physics, chemistry and biology are sciences where it is very common to find models reflecting the interaction between dynamical systems. The behaviour of each system as an isolated object can be identical or not and the interaction mechanisms can be very varied. Usually these models are referred to as *coupled systems*.

Certainly many different questions arise in this context. For instance, there is a great interest in the dynamical properties which depend on the architecture of the coupling, more than on the internal behaviour of each element. Synchronization problems are also of the highest interest and the literature related with this topic is very extensive.

We are particularly concerned about the possibility of creating complexity by coupling, with elementary interaction rules, systems exhibiting simple dynamics: either stationary or periodic. One can find many examples in the literature showing numerically how indeed chaotic behaviour can arise by *simple coupling of simple systems* (see for instance [2, 4, 18, 19, 24]).

As already mentioned, the term "coupling system" can refer to many different types of interaction. We consider specifically a general model of identical ordinary

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differential equations linearly coupled by diffusion:

$$\mathbf{u}_i' = F(\mathbf{u}_i) + \sum_{j=1}^{m} a_{ij} D(\mathbf{u}_j - \mathbf{u}_i), \quad i = 1, \dots, m, \tag{1.1}$$

where $\mathbf{u}_i \in \mathbb{R}^k$ for each $i = 1, \dots, m$, D is a $k \times k$ diagonal matrix with positive entries and coefficients a_{ij} can be either 0 or 1 and satisfy that $a_{ij} = a_{ji}$. Moreover, F is a C^∞ vector field in $\mathbb{R}^k$, maybe depending on some fixed parameters.

The seminal work of Alan Turing [25], where he studied the arising of oscillatory behaviour in a ring of diffusively coupled linear systems, led Smale [23] to wonder whether globally attracting periodic orbits could be generated in a coupling of the type (1.1) when the internal dynamics reduces to a globally attracting equilibrium point. He provided a concrete example with $m = 2$ (two interacting systems) and $k = 4$. Examples, again with $m = 2$, with $k = 3$ and $k = 2$ were obtained in [13] and [1], respectively.

With this motivation it is very natural to wonder which other behaviour can be generated when elementary dynamics (globally attracting stationary or periodic orbits) are coupled by diffusion. In particular it is interesting to know whether chaos can emerge with such assumptions. Positive answers based on numerical simulations are present in the literature (see [2, 4, 18, 24]). Particularly, the numerical evidences supplied in [2, 24] correspond to a model consisting of two brusselators linearly coupled by diffusion:

$$\begin{cases} x_1' = A - (B+1)x_1 + x_1^2 y_1 + \lambda_1(x_2 - x_1), \\ y_1' = Bx_1 - x_1^2 y_1 + \lambda_2(y_2 - y_1), \\ x_2' = A - (B+1)x_2 + x_2^2 y_2 + \lambda_1(x_1 - x_2), \\ y_2' = Bx_2 - x_2^2 y_2 + \lambda_2(y_1 - y_2). \end{cases} \tag{1.2}$$

In the sequel we will refer to the above system as the *two-coupled brusselators model.* Note that when $\lambda_1 = \lambda_2 = 0$ we have indeed two uncoupled copies of the system which is known in the literature as "the brusselator". It models a chemical reaction and due to that reason only the phase portrait restricted to the first quadrant is of interest. It can be proven that such region is invariant for the forward flow and only contains bounded orbits. On the other hand, parameters A and B are both strictly positive. A Hopf bifurcation takes place when $B = A^2 + 1$. In the first quadrant there is a unique globally attracting equilibrium point if $B < A^2 + 1$ and a unique globally attracting periodic orbit if $B > A^2 + 1$.

In [7] we proved, with analytical arguments, that the two-coupled brusselators model contains strange attractors. More precisely, the following result was obtained:

Theorem 1.1. *There exists a point* $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$ *in the parameter space such that, arbitrarily nearby, there are values* $(A, B, \lambda_1, \lambda_2)$ *for which, restricted to a normally attracting 3-dimensional invariant manifold, system (1.2) has Shil'nikov homoclinic orbits and hence strange attractors.*

The main goal of this paper is to provide examples of the chaotic behaviour predicted by the theoretical results.

Analytical results showing the existence of chaotic behaviour in a given system are very rare in the literature. It is certainly well known that, under generic assumptions, the occurrence of some global configuration implies the existence of strange attractors. The most simple of such configurations is a Shil'nikov homoclinic orbit (see [12], [21] and [22]). Unfortunately, the detection of such configuration in a given system is again a very involved task. However, it is known that when certain singularities are generically unfolded by a given family of vector fields, then Shil'nikov homoclinic orbits are generically unfolded too (see [14] and [15]). Therefore, the detection of the appropriate singularities turns into the most simple tool to prove analytically the existence of strange attractors and consequently of chaos.

To be more precise, in [15] it was proved that Shil'nikov configurations occur in any generic unfolding of the nilpotent singularity of codimension three in $\mathbb{R}^3$, that is, any singularity that can be reduced to the following normal form:

$$y\frac{\partial}{\partial x} + z\frac{\partial}{\partial y} + (ax^2 + bxy + cxz + dy^2 + O(\|(x, y, z)\|^3))\frac{\partial}{\partial z},$$

with $a \neq 0$.

Remark 1.2. A 3-dimensional nilpotent singularity of codimension 3 involves much more dynamical richness than that mentioned in this paper (see [9] and [10]). It should be noticed that, in fact, many aspects of its bifurcation diagram remain still unexplained.

The point $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$ given in Theorem 1.1 corresponds to values where system (1.2) has a 4-dimensional nilpotent singularity of codimension 4 which is generically unfolded inside the family. After proving that any generic unfolding of an n-dimensional nilpotent singularity of codimension n contains generic unfoldings of $(n-1)$-dimensional nilpotent singularities of codimension $n-1$, Theorem 1.1 follows.

Remark 1.3. The search for more singularities unfolding chaotic dynamics is still in progress (see [5, 6, 11] for the case of the Hopf-zero singularity). On the other hand their appearance as organizing center in systems arising from applications is common in the literature. Nevertheless they are rarely used when working with coupled systems. In this sense we believe that more examples, and also canonical models, have to be studied to show, in that context, the role of singularities to explain chaotic dynamics and even synchronization phenomena.

In Section 2 we will recall the generic conditions described in [7] with the aim to supply here an error analysis. The point $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$ given in Theorem 1.1, although algebraically determined by two equations, has to be estimated by a numerical method. Hence generic conditions are only checked up to some small error, whose analysis was not included in [7]. In Section 3 we will provide a numerical study of a region of chaotic dynamics linked to our theoretical results.

2 Singularities in the two coupled brusselators model

To study (1.2) it is more convenient to introduce the following variables:

$$\xi_1 = (x_2 - x_1)/2, \quad \xi_2 = (y_2 - y_1)/2, \quad \eta_1 = (x_2 + x_1)/2 \text{ and } \eta_2 = (y_2 + y_1)/2.$$

In the new coordinates (1.2) takes the form

$$\begin{cases} \xi_1' = -(B+1)\xi_1 + (\eta_1^2 + \xi_1^2)\xi_2 + 2\eta_1\eta_2\xi_1 - 2\lambda_1\xi_1, \\ \xi_2' = B\xi_1 - (\eta_1^2 + \xi_1^2)\xi_2 - 2\eta_1\eta_2\xi_1 - 2\lambda_2\xi_2, \\ \eta_1' = A - (B+1)\eta_1 + (\eta_1^2 + \xi_1^2)\eta_2 + 2\xi_1\xi_2\eta_1, \\ \eta_2' = B\eta_1 - (\eta_1^2 + \xi_1^2)\eta_2 - 2\xi_1\xi_2\eta_1. \end{cases} \tag{2.1}$$

Note that the flow is invariant under the symmetry

$$(\xi_1, \xi_2, \eta_1, \eta_2) \to (-\xi_1, -\xi_2, \eta_1, \eta_2).$$

On the invariant plane $\{\xi_1 = 0, \xi_2 = 0\}$ the restricted system is given by the brusselator equations. Therefore, for all parameter values, there is a unique equilibrium point at $(0, 0, A, B/A)$ on that plane which undergoes a Hopf bifurcation when $B = A^2 + 1$. We refer to that point as the trivial singularity.

It easily follows (see [7] for details) that for every equilibrium point of the system the following relations hold

$$\xi_2 = -(1 + 2\lambda_1)\xi_1/2\lambda_2, \quad \eta_1 = A, \quad \eta_2 = (AB - 2A\xi_1\xi_2)/(A^2 + \xi_1^2)$$

and the ξ_1 coordinate is a solution of the equation:

$$\xi_1 \left[(A^2 + \xi_1^2)^2 + (A^2 + \xi_1^2)p + q\right] = 0,$$

with

$$p = [2\lambda_2(B + 2\lambda_1 + 1) - 4A^2(1 + 2\lambda_1)]/(1 + 2\lambda_1)$$

and

$$q = [4A^2(A^2(1 + 2\lambda_1) - B\lambda_2)]/(1 + 2\lambda_1).$$

Saddle-node bifurcations occur when $\xi_1 = \pm\sqrt{-p/2 - A^2}$ and $p^2 - 4q = 0$. Computing the characteristic polynomial of the Jacobian at a saddle-node bifurcation point we get

$$r^4 + c_3 r^3 + c_2 r^2 + c_1 r$$

with:

$$\begin{aligned} c_1 &= 4(A + 2\lambda_1)^2 \Big[-B^3 + B^2(-1 + 2\lambda_1) + (1 + 2\lambda_1)^2(1 + 6\lambda_1) \\ &\quad + B(1 + 8A^2 + 12\lambda_1 + 20\lambda_1^2)\Big] / (1 + B + 2\lambda_1)^3, \\ c_2 &= \Big[32A^4B(1 + 2\lambda_1)^2 + (1 + B + 2\lambda_1)^4 (1 + 3\lambda_1) \\ &\quad - 8A^2 \Big(B^3\lambda_1 + (1 + 2\lambda_1)^3 (2 + 5\lambda_1) + B(1 + 2\lambda_1)^2 (4 + 9\lambda_1) \\ &\quad + B^2 \left(2 + 9\lambda_1 + 10{\lambda_1}^2\right)\Big)\Big] / (1 + B + 2\lambda_1)^3, \\ c_3 &= \Big[-(1 + B + 2\lambda_1)^2 (1 + B + 4\lambda_1) \\ &\quad + 4A^2 \left(B^2 + (1 + 2\lambda_1)^2\right)\Big] / (1 + B + 2\lambda_1)^2. \end{aligned}$$

From the saddle-node condition and from the equation $c_1 = 0$ we easily get

$$\lambda_2 = \left(\frac{2A(1+2\lambda_1)}{1+B+2\lambda_1}\right)^2, \quad A = \frac{\sqrt{-1+B-6\,\lambda_1}\,(1+B+2\,\lambda_1)}{2\,\sqrt{2}\,\sqrt{B}}. \tag{2.2}$$

After substituting A and λ_2 as given above, one can see that there is a unique solution $(\hat{B}, \hat{\lambda}_1)$ for the system given by $c_2 = c_3 = 0$. We compute such solution with the Newton method and obtain that, for the parameter values

$$\begin{aligned} \hat{A} &= 2.6021429374428 \pm 3.e^{-13}, \\ \hat{B} &= 11.2982916303634 \pm 1.e^{-13}, \\ \hat{\lambda}_1 &= 1.2506765845779 \pm 1.e^{-13}, \\ \hat{\lambda}_2 &= 1.5159732649714 \pm 2.e^{-13}, \end{aligned}$$

the two coupled-brusselator model has a four dimensional nilpotent singularity at the point

$$\begin{aligned} \hat{x}_1 &= 1.99933463252094 \pm 4.e^{-14}, \\ \hat{y}_1 &= 5.12301336349842 \pm 1.2e^{-13}, \\ \hat{x}_2 &= 3.2049512423647 \pm 6.e^{-13}, \\ \hat{y}_2 &= 3.7307429207399 \pm 6.e^{-13}. \end{aligned}$$

It was checked in [7] that the linear part at the singularity is linearly conjugate to

$$u_2\frac{\partial}{\partial u_1} + u_3\frac{\partial}{\partial u_2} + u_4\frac{\partial}{\partial u_3}.$$

It was also proved that, after translating the singularity at the origin and in the appropriate coordinates, any vector field with such singularity could be written as

$$u_2\frac{\partial}{\partial u_1} + u_3\frac{\partial}{\partial u_2} + u_4\frac{\partial}{\partial u_3} + f(u)\frac{\partial}{\partial u_4},$$

with $u = (u_1, u_2, u_3, u_4)$ and $f(u) = O(\|u\|^2)$. If

$$\frac{\partial^2 f}{\partial u_1^2}(0) \neq 0 \tag{2.3}$$

the singularity is of codimension four. In such a case any unfolding can be written as

$$\begin{aligned} &u_2\frac{\partial}{\partial u_1} + u_3\frac{\partial}{\partial u_2} + u_4\frac{\partial}{\partial u_3} \\ &+(a_1(\mu) + a_2(\mu)u_2 + a_3(\mu)u_3 + a_4(\mu)u_4 + u_1^2 + h(\mu, u))\frac{\partial}{\partial u_4}, \end{aligned}$$

where we assume that $\mu \in \mathbb{R}^4$, the coefficients $a_i(\mu)$, with $i = 1, 2, 3, 4$, represent exact coefficients in a Taylor expansion with respect to u and h is $O(\|(\mu, u)\|^2)$ and also $O(\|(u_2, u_3, u_4)\|^2)$.

Let $a(\mu) = (a_1(\mu), a_2(\mu), a_3(\mu), a_4(\mu))$. The unfolding is generic if

$$\text{Det}\,[D_\mu a(0)] \neq 0. \tag{2.4}$$

In such a case it follows from the results in [7] that the unfolding contains two generic bifurcation curves of three dimensional nilpotent singularities of codimension three and, consequently, the existence of strange attractors.

In [7] the left-hand sides of expressions (2.3) and (2.4) were provided without any discussion about the estimation of the error due to the use of approximate values for parameters and variables. Here we include such estimation. Note that in [7] explicit algebraic formulas were provided in order to check the generic conditions.

Remark 2.1. *In general, given a function $y = f(x_1, \dots, x_n)$ and assuming that we know approximate values*

$$x_i = \bar{x}_i \pm \Delta x_i,$$

for $i = 1, \dots, n$, we will get an approximate value $y = f(\bar{x}) \pm \Delta y$ with absolute error

$$\Delta y = \left| \frac{\partial f}{\partial x_1} \right|_{\bar{x}} \Delta x_1 + \cdots + \left| \frac{\partial f}{\partial x_n} \right|_{\bar{x}} \Delta x_n,$$

where $\bar{x} = (\bar{x}_1, \dots, \bar{x}_n)$.

Using the above approach, that is, estimating the increase of the error in each algebraic computation, we get that the left hand sides in expressions (2.3) and (2.4) are

$$175.163090114 \pm 3.e^{-9}$$

and

$$-365263.4408 \pm 6.e^{-4},$$

respectively. Therefore the required generic conditions are satisfied.

Remark 2.2. Although we only mention the nilpotent singularities arising in the two-coupled brusselators model, it should be noticed that there appear others with a very rich unfolding. At the trivial singularity one can find pitchfork-Hopf singularities of codimension two and three. Note that pitchfork-Hopf singularities have been studied in the literature (see [16] for the codimension two cases and [3], and references therein, for the codimension three cases) but their unfoldings are not yet completely understood. Of course there also appear Hopf-Hopf singularities at the trivial equilibrium point when $\lambda_1 = \lambda_2 = 0$ and $B = A^2+1$. In the specific context of coupled systems they were studied in [4]. For the nontrivial singularities we should underline that most of the dynamics in the unfolding of the 4-dimensional nilpotent singularity of codimension four is completely unknown. There also exist Bogdanov-Takens-Hopf singularities. Their unfolding is again only partially understood and the only reference, as far as we know, is [17].

3 Chaotic dynamics: numerical results

According to Theorem 1.1, arbitrarily near $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$ there are parameter values $(A, B, \lambda_1, \lambda_2)$ for which the system (1.2) has Shil'nikov homoclinic orbits and hence strange attractors.

We shall compute Lyapunov exponents for family (1.2) with parameter values near $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$ to find examples of those strange attractors whose existence has been proven in [7]. Using our own algorithms (usual numerical integration procedure for Fortran 90 with a Taylor series method of order 25 and variable step-sizes for all numerical integration of the ODEs), we will show that small regions with a positive value of the maximum Lyapunov exponent appear near the bifurcation point $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$.

Before we present the numerical results we just briefly comment on how they are done. We first choose a suitable range of parameters. Note that the strange attractors we are looking for are related with Shil'nikov homoclinic orbits. Therefore, we will reduce our study to those parameter values for which the system has a saddle-focus equilibrium point with eigenvalues ν and $\rho \pm i\omega$ such that the Shil'nikov condition, $\nu > |\rho|$, is satisfied. Additionally, we fix a point,

$$\alpha = (\bar{A}, \bar{B}, \bar{\lambda}_1, \bar{\lambda}_2) \approx (2.69201, 11.51650, 1.26066, 1.58948),$$

on the bifurcation curve TZ of 3-dimensional nilpotent singularities of codimension 3 where the non-zero eigenvalue is negative. Of course, α is chosen close to $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$.

Remark 3.1. *Notice that the curve TZ is explicitly determined by the saddle-node condition $p^2 - 4q = 0$, the equations $c_1 = c_2 = 0$ and the condition $c_3 \neq 0$. Expressions for p, q, c_1, c_2 and c_3 are given in Section 2.*

At α we take the hyperplane S which is orthogonal to TZ. On S λ_2 can be written as a function of (A, B, λ_1) and therefore, in the sequel, we only have to work with three parameters. We finally consider a 1-parameter family of planes in S

$$T_\epsilon = \left\{ (A + \epsilon, B, \lambda_1) \in \mathbb{R}^3 : (A, B, \lambda_1) \in T_\beta \right\},$$

with ϵ small and where T_β denotes the tangent plane to the saddle-node bifurcation surface (restricted to S) at $\beta = (\bar{A}, \bar{B}, \bar{\lambda}_1)$. Our numerical results are obtained for parameter values near β on T_ϵ with $\epsilon = -1.e^{-3}$ and verifying the Shil'nikov condition.

On each plane T_ϵ we get A as a function of (B, λ_1) and hence we have reduced the study to only two parameters. The results presented in this paper to illustrate how change in dynamics through a chaotic region correspond to $\lambda_1 = 1.205$ and $B \in (11.475, 11.477)$. All the tests have been done for inicial conditions near the 1-dimensional unstable manifold of a saddle-focus equilibrium point. Some computations of Lyapunov exponents are shown in Table 1.

The spectrum of the Lyapunov exponents which correspond to a strange atractor are of type $(+, 0, -, -)$. In Fig. 1, we show the typical bifurcation diagram of attractors for $B \in (11.47500, 11.47605)$. There we can see a region with an infinite sequence of period-doubling bifurcations followed by a chaotic region.

	B	μ_1	μ_2	μ_3	μ_4
(a)	11.47520	0.000	-0.035	-0.571	-3.064
(b)	11.47540	0.000	-0.003	-0.605	-3.053
(c)	11.47560	0.000	-0.019	-0.597	-3.042
(d)	11.47570	0.000	-0.002	-0.616	-3.036
(e)	11.47580	0.031	0.000	-0.651	-3.031
(f)	11.47590	0.033	0.000	-0.665	-3.024
(g)	11.47610	0.053	0.000	-0.692	-3.012
(h)	11.47630	0.055	0.000	-0.676	-3.004
(i)	11.47650	0.066	0.000	-0.690	-2.993
(j)	11.47670	0.000	-0.004	-0.550	-2.993
(k)	11.47690	0.074	0.000	-0.642	-2.980
(l)	11.47700	0.000	-3.711	-20.31	-22.36

Table 1: Lyapunov exponents of system (1.2) for some parameter values on T_ϵ with $B \in (11.475, 11.477)$ and $\lambda_1 = 1.205$.

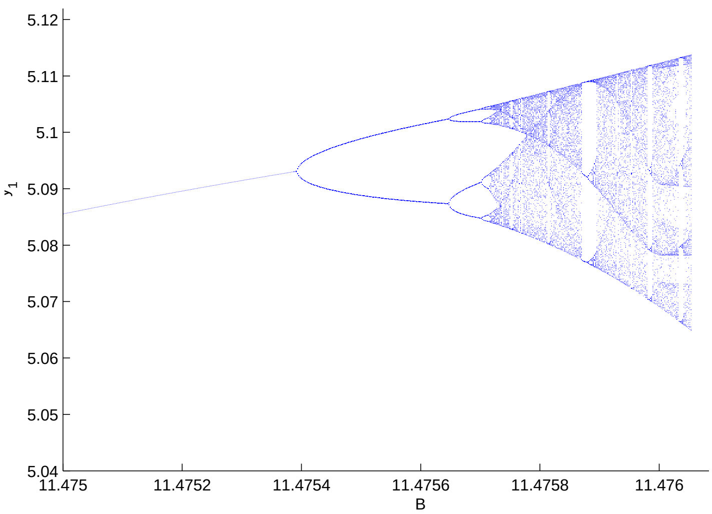


Figure 1: Bifurcation diagram of attractors obtained by plotting the values of y_1 for $B \in (11.47500, 11.47605)$.

Numerically computed examples of attractors (projected on (x_2, y_2, x_1) space) for various values of parameter B are shown in Fig. 2. Figures 2$(i - ii)$ correspond to two periodic orbits whose Lyapunov exponents are given in Table 1, see cases (a) and (d). Figures 2$(iii - v)$ show three examples of strange attractors we have found near the bifurcation point $(\hat{A}, \hat{B}, \hat{\lambda}_1, \hat{\lambda}_2)$. The maximum Lyapunov exponent of these attractors is given in Table 1 cases (f), (h) and (k), respectively. The attractor shown in Fig. 2(vi) is again a periodic orbit. It is remarkable that in this case the periodic orbit is contained in the invariant plane $\Pi \equiv \{x_1 = x_2, y_1 = y_2\}$ and therefore a synchronization phenomenon appears. To illustrate it we show evolution over time of variables (x_1, x_2) and (y_1, y_2) in Fig. 3(2). We can also see in Fig. 3(1) how variables of a strange attractor evolve over time. All graphics in this paper have been done using Matlab [20].

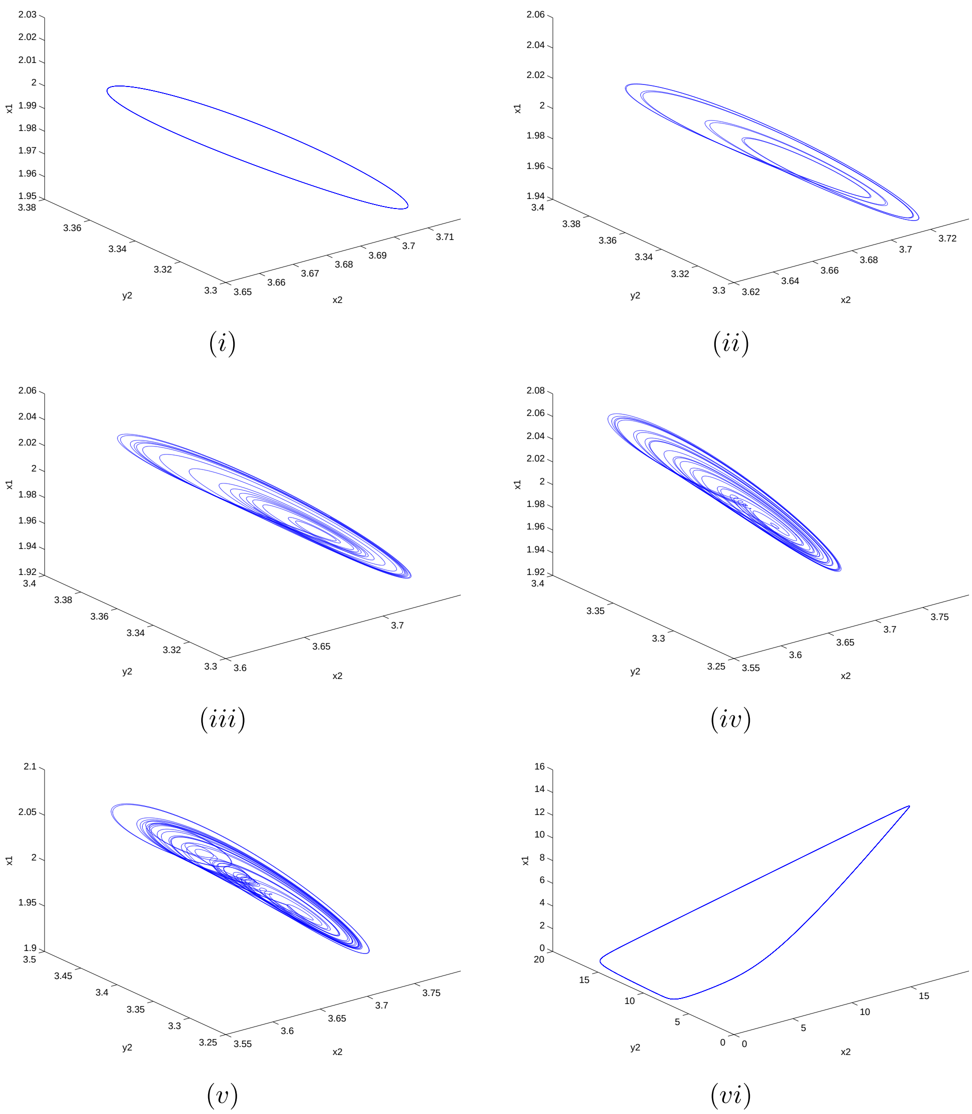
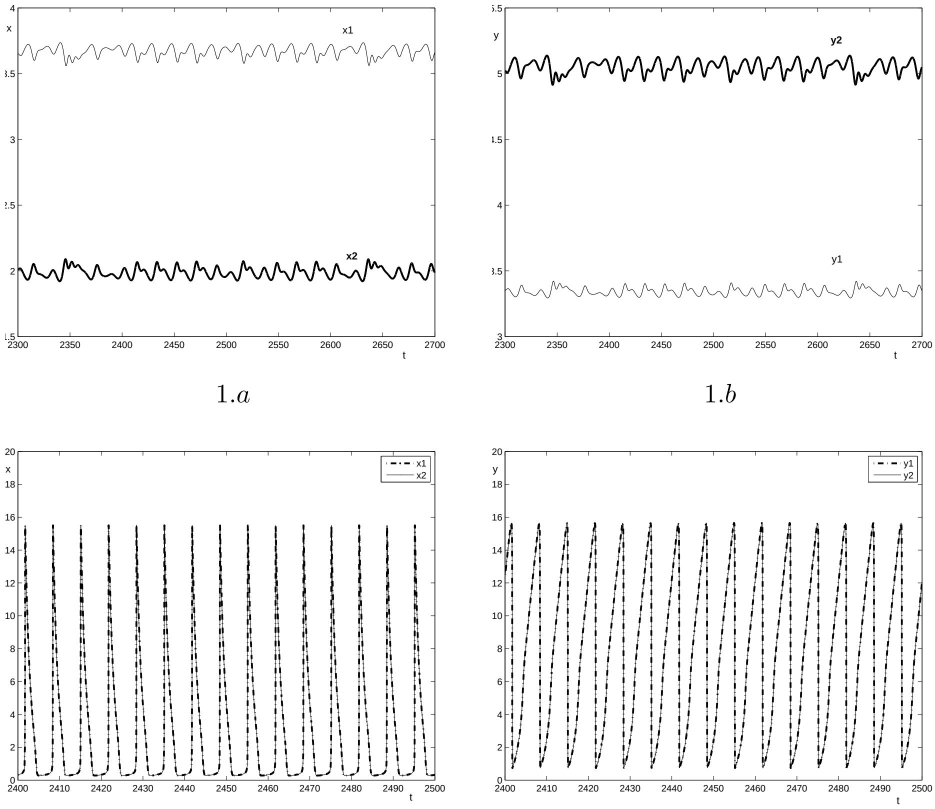


Figure 2: Projection of attractors on the (x_2, y_2, x_1) space at different values of B: (i) 11.47520, (ii) 11.47570, (iii) 11.47590, (iv) 11.47630, (v) 11.47690, and (vi) 11.47700. (i) and (ii) are periodic attractors; $(iii) - (v)$ are chaotic attractors; and (vi) is a periodic attractor on the invariant plane Π.



1.*a* 1.*b*

2.*a* 2.*b*

Figure 3: Evolution over time of variables (x_1, x_2) and (y_1, y_2) at different values of B: 1.(*a*-*b*) 11.47690, 2.(*a*-*b*) 11.47700.

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