A method to determine the dimension of long-time dynamics in multi-scale systems

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Abstract

Modeling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be large. The problem of determination of the minimal number of phase variables needed to describe the characteristic behavior of large scale systems is extensively addressed in current chemical kinetics literature from different point of views. Only for a few of these approaches there exists a mathematical justification.

In this paper we describe and justify a procedure allowing directly to determine how many and which state variables are essential in a neighborhood of a given point of the extended phase space. This method exploits the wide range of characteristic time-scales in a chemical system and its mathematical justification is based on the theory of invariant manifolds. The procedure helps to get chemical insight into the intrinsic dynamics of a complex chemical process.

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1 Introduction.

Modeling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be quite large. One of the important questions extensively addressed in current chemical kinetics literature is related to the problem of determination of the minimal number of phase variables needed to describe the characteristic behavior of large scale systems (see, e.g., Heard et al. [1], and Lowe and Tromlin [2]). There are different approaches to reduce models describing complex chemical processes. The first, most frequently used approach is based on the presence of a wide range of characteristic time-scales in a chemical system. Its simplest variants are the quasi-steady state assumption (QSSA) (see, e.g., Schneider and Wilhelm [3], Segal [4] and Segal and Slemrod [5], and the quasi-equilibrium assumption (QEA) (see, e.g., Heinrich and Schuster [6]). The method of intrinsic low dimensional manifolds (see, e.g., Maas [7], Maas and Pope [8], and Schmidt et al. [9]) also belongs to that type of reduction methods. Other procedures involve application of conservation relations, lumping of species (molecular and structural lumping, see Atkinson et al. [10] and Gery et al. [11]), sensitivity analysis (see Turányi [12]) and replacing differential equations by input-output relations (special case of the general procedure called repro-modelling (see Lowe and Tomlin [2] and Turányi [13]). Only for a few of these approaches there exists a mathematical justification.

In what follows we propose a method to approximate a number which characterizes the dimension of the underlying long-time dynamics in a multi-scale system. We estimate this dimension from above at different points in the extended phase space. Our estimate is based on the method of integral manifolds which can be also used to justify the QSSA and QEA. Knowing only the number of phase variables responsible for underlying dynamics in a chemical system can help to make conclusions about its qualitative behavior (oscillations, chaos), as well as to get chemical insight into intrinsic dynamics of the process.
Let us introduce some notions related to the topic of our discussion. We assume that the adequate mathematical model can be written in the form of a system of ordinary differential equations

$$\frac{dz}{dt} = h(z,t), \tag{1.1}$$

where z is an n-vector. In the case when different characteristic time scales related to fast and slow reactions are present in the chemical kinetics system, the mentioned above approach, QSSA, can be used to reduce the number of differential equations in system (1.1). For that the derivatives of fast variables are assumed to be zero. Consequently, we arrive at a differential-algebraic system which represents under certain additional conditions a dynamical system on the constrained manifold. This procedure requires some knowledge of the underlying chemistry telling us which variables are slow and which are fast.
In case when (1.1) can be rewritten as a singularly perturbed system

$$\begin{aligned} \frac{dx}{dt} &= f(x,y,t,\varepsilon), \\ \varepsilon\frac{dy}{dt} &= g(x,y,t,\varepsilon), \end{aligned} \tag{1.2}$$

where $x \in R^m, y \in R^k, n = m + k$, and ε is a small positive parameter, the problem of distinguishing fast and slow variables can be easily solved. Setting $\varepsilon = 0$ in (1.2) we get the differential-algebraic system

$$\begin{aligned} \frac{dx}{dt} &= f(x, y, t, 0), \\ 0 &= g(x, y, t, 0), \end{aligned} \tag{1.3}$$

which is called the *degenerate system* for (1.2). If we are able to solve the second equation with respect to y, $y = \varphi(x, t)$, then we can substitute y by $\varphi(x, t)$ in the first equation and get the differential system

$$\frac{dx}{dt} = f(x, \varphi(x, t), t, 0), \tag{1.4}$$

which is said to be the *reduced degenerate system* for (1.2) and whose state space has the dimension $m = n - k$. The claim that for sufficiently small positive ε the qualitative behavior of system (1.2) near the surface $y = \varphi(x, t)$ is determined by the behavior of system (1.4) can be justified by means of the theory of invariant manifolds for singularly perturbed systems (see, e.g., Fenichel [14] and Strygin and Sobolev [15]) under the condition that the spectrum of the Jacobian $g_y(x, \varphi(x, t), t, 0)$ is located in the left half plane for all (x, t) under consideration.
One important problem in studying (1.1) is to find out which variables are fast at the point $z = z_0$ and at the time $t = t_0$. To treat this problem we consider first the spectrum σ^0 of the Jacobian J^0 of the right hand side of (1.1) at (z_0, t_0). A crucial step is to divide σ^0 into two disjoint parts, $\sigma^0 = \sigma^0_{-\nu} \cup \sigma^0_r$, where the real parts of all eigenvalues of $\sigma^0_{-\nu}$ are less than $-\nu$, $\nu > 0$. Then we look for a transformation such that J^0 is equivalent to a matrix $diag(S^0_{11}, S^0_{22})$ with $\sigma(S^0_{22}) = \sigma^0_{-\nu}$. The main goal of this paper is to derive conditions guaranteeing that the splitting of the spectrum σ^0 into $\sigma^0_{-\nu}$ and σ^0_r implies a splitting of the variables into fast and slow. To this end we prove the existence of a locally invariant manifold of system (1.1) near (z_0, t_0) which is exponentially attracting.
The approach to use the spectrum of the Jacobian J^0 in order to find out which variables are fast has been applied also by U. Maas [7] and by Maas and Pope [8] and by P. Deuflhard and J. Heroth [16] in case of an autonomous system. Deuflhard and Heroth use the method of asymptotic expansion of the solution to an initial value problem of a singularly perturbed system to get information on the local error of the approximation of (1.2) by the differential-algebraic system (1.3), whereas Maas gives no mathematical justification for the introduction of his so-called 'intrinsic manifolds'.
The paper is organized as follows. In section 2 we prove a modification of Gronwall's Lemma and recall some basic facts about the real Schur decomposition. In section 3 we prove a theorem about the existence of an integral manifold for a singularly perturbed system with a special structure. Here, particular attention is devoted to the estimate of the ε-interval for which the manifold exists. Our algorithm for determining the points in the (x, t)-space where the dimension of the state space of the reaction system (1.1) can be reduced is presented in section 4. In section 5 we illustrate our approach by some examples. The first example is a reaction scheme due to P. Duchêne and P. Rouchon [17], the second represents the famous Oregonator [18], the last one is related to a troposcopic chemistry model which exhibits oscillations and

chaos (see, e.g., Field et al. [19] and Kalachev and Field [20]). Short conclusion with a brief discussion of the results is presented in the last section.

2 Preliminaries

In this section we prove a modification of Gronwall's lemma and recall some basic facts about the block diagonalization of a matrix by means of a real Schur decomposition which will be used to derive a singularly perturbed system with a special structure.
The following lemma is known as Gronwall's lemma.
Lemma 2.1 *Let k_1 be a positive constant, let k_2 and k_3 be nonnegative constants. Let f be a continuous nonnegative function defined on the interval $\alpha \le t \le \beta$ satisfying for all t the inequality*

$$f(t) \le k_1 \int_\alpha^t f(s)ds + k_2(t-\alpha) + k_3. \tag{2.1}$$

Then, for $\alpha \le t \le \beta$, we have

$$f(t) \le \left(\frac{k_2}{k_1} + k_3\right) e^{k_1(t-\alpha)} - \frac{k_2}{k_1}.$$

Under the assumptions of this lemma, the right hand side of (2.1) is monotone increasing in t. The following lemma is concerned with a similar inequality but under the assumption that the right hand side is monotone decreasing.
Lemma 2.2 *Let the constants k_1, k_2, k_3 and the function f be as above, and let f now satisfies*

$$f(t) \le k_1 \int_t^\beta f(s)ds + k_2(\beta - t) + k_3. \tag{2.2}$$

Then, for $\alpha \le t \le \beta$, it holds

$$f(t) \le \left(\frac{k_2}{k_1} + k_3\right) e^{k_1(\beta-t)} - \frac{k_2}{k_1}. \tag{2.3}$$

Proof. We introduce the nonnegative function χ by $\chi(t) := f(t) + k_2/k_1$, and the nonnegative constant $k_0 := k_2/k_1 + k_3$. Then, from (2.2) we get that χ satisfies

$$\chi(t) \le k_1 \int_t^\beta \chi(s)ds + k_0. \tag{2.4}$$

From (2.4) we derive

$$\frac{\chi(t)}{k_1 \int_t^\beta \chi(s)ds + k_0} \le 1.$$

Multiplication by k_1 and integration yields

$$\int_t^\beta \frac{k_1\chi(\xi)}{k_1 \int_\xi^\beta \chi(s)ds + k_0} d\xi \le k_1 \int_t^\beta d\xi,$$

which is equivalent to

$$k_1 \int_t^\beta \chi(s)ds + k_0 \leq k_0 e^{k_1(\beta - t)}.$$

Using (2.4) we get

$$\chi(t) \leq k_0 e^{k_1(\beta - t)}.$$

Taking into account the definition of χ we have

$$f(t) \leq \left(\frac{k_3}{k_2} + k_3\right) e^{k_1(\beta - t)} - \frac{k_2}{k_1}.$$

To prove the existence of an attracting invariant manifold $y = \bar{r}(x, t, \varepsilon)$ for system (1.2) we need that g_y has eigenvalues with sufficiently large negative real parts. The following procedure aims to find at a given point (z_0, t_0) in the space of motion of system (1.1) a coordinate transformation such that in the new coordinates $h_z(z_0, t_0)$ has a block-diagonal structure where one block has only eigenvalues with negative real parts. This transformation contributes also to finding out the fast variables in (1.1). The first step of this procedure is the, so-called, real Schur decomposition. According to Golub and van Loan [21] Chapt. 7.4.1 we have:

Proposition 2.1 *For any real $n \times n$-matrix M there exists an orthogonal $n \times n$-matrix Q such that $Q^T M Q$ has the structure*

$$Q^T\, M\, Q =: R = \begin{pmatrix} R_{11} & R_{12} & \cdots & R_{1l} \\ 0 & R_{22} & \cdots & R_{2l} \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & R_{ll} \end{pmatrix},$$

where each R_{ii} is either a (1×1)–matrix or a (2×2)–matrix having complex conjugate eigenvalues.

The matrix R represents a real Schur decomposition. To get an ordering of the eigenvalues of R according to the magnitude of their real parts we can apply the, so-called, Givens- rotations (c.f. Golub and van Loan [21], Chapt. 7.6.2). Hence, without loss of generality, we may assume the ordering $Re\ \sigma(R_{ii}) \geq Re\ \sigma(R_{i+1\ i+1})$ for $i = 1, \ldots, l-1$.
Now we split the spectrum $\sigma(R)$ of R by means of the splitting parameter $\nu > 0$ into two disjoint sets

$$\begin{aligned} \sigma_{-\nu} &:= \{\lambda \in \sigma(R) \,:\, Re\,\lambda < -\nu\}, \\ \sigma_r &:= \{\lambda \in \sigma(R) \,:\, Re\,\lambda \geq -\nu\}. \end{aligned}$$

Then R may be written in the form

$$R = \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix},$$

where S_{11} and S_{22} are upper triangular matrices with possible non-vanishing entries on the first sub-diagonal related to complex conjugate eigenvalue pairs such that $\sigma_r = \sigma(S_{11})$ and $\sigma_{-\nu} = \sigma(S_{22})$.
The transformation of R into a block-diagonal matrix can be performed as follows. We determine the sub-matrix Z in the $n \times n$-matrix Y,

$$Y = \begin{pmatrix} I & Z \\ 0 & I \end{pmatrix},$$

in such a way that we have

$$Y^{-1} R Y = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix}.$$

From

$$\begin{aligned} Y^{-1} R Y &= \begin{pmatrix} I & -Z \\ 0 & I \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix} \begin{pmatrix} I & Z \\ 0 & I \end{pmatrix} \\ &= \begin{pmatrix} S_{11} & S_{11} Z - Z S_{22} + S_{12} \\ 0 & S_{22} \end{pmatrix} = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix} \end{aligned}$$

we obtain the following matrix equation for Z

$$S_{11} Z - Z S_{22} = -S_{12}.$$

If we set

$$T = QY,$$

then we have

$$S := T^{-1} M T = Y^{-1} Q^T M Q Y = Y^{-1} R Y = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix}.$$

which has the block-diagonal structure we are looking for.

3 Existence of an integral manifold of a singularlyperturbed system

Our goal is a local reduction of the state space of system (4.1) in a neighborhood $\mathcal{N}$ of a given point (z_0, t_0) by means of a local exponentially attracting invariant manifold. To this purpose we prove in this section a theorem on the existence of a unique global integral manifold $\mathcal{M}_\varepsilon$ for the following singularly perturbed system with a special structure.

$$\begin{aligned} \frac{du_1}{dt} &= f(u_1, u_2, t), \\ \varepsilon \frac{du_2}{dt} &= B u_2 + \varepsilon g(u_1, u_2, t) \end{aligned} \tag{3.1}$$

The intersection of the global integral manifold $\mathcal{M}_\varepsilon$ with the neighborhood $\mathcal{N}$ yields the local integral manifold of interest to us. The proof of the existence of $\mathcal{M}_\varepsilon$ requires that the functions f and g in (3.1) are defined everywhere. To satisfy this condition we modify f and g outside $\mathcal{N}$ so that they vanish there identically. Consequently, the assumption (A_2) on f and g presented below can be considered as local assumption concerning the neighborhood $\mathcal{N}$.
The method to establish the existence of $\mathcal{M}_\varepsilon$ is basically the same as in Strygin and Sobolev [15] but our special concern is to give an estimate of the ε-interval for which the global integral manifold exists.
We consider system (3.1) for sufficiently small ε $(0 \le \varepsilon \le \varepsilon^*)$ under the following assumptions:

(A_1). $f : G := R^m \times R^k \times R \to R^m$ and $g : G \to R^k$ are continuous and continuously differentiable with respect to all variables.

(A_2). Let $|.|$ be the Euclidean norm. There are positive constants $c_1, c_2, c_{41}, c_{42}, c_{51}, c_{52}$ such that f and g satisfy in G the conditions

$$|f(u_1, u_2, t)| \le c_1,$$
$$|g(u_1, u_2, t)| \le c_2, \tag{3.2}$$
$$|f(u_1, u_2, t) - f(\tilde{u}_1, \tilde{u}_2, t)| \le c_{41}|u_1 - \tilde{u}_1| + c_{42}|u_2 - \tilde{u}_2|, \tag{3.3}$$
$$|g(u_1, u_2, t) - g(\tilde{u}_1, \tilde{u}_2, t)| \le c_{51}|u_1 - \tilde{u}_1| + c_{52}|u_2 - \tilde{u}_2|, \tag{3.4}$$

for all $(u_1, u_2, t), (\tilde{u}_1, \tilde{u}_2, t) \in G$.

(A_3). B is a constant $k \times k$-matrix whose eigenvalues λ_i have negative real parts, i.e., there is a positive number γ such that $Re\ \lambda_i < -\gamma < 0\ \forall\, i$.

For $\varepsilon = 0$, (3.1) has the integral manifold $u_2 \equiv 0$. It is natural to expect that, for sufficiently small ε, (3.1) has an integral manifold $\mathcal{M}_\varepsilon$ near $u_2 \equiv 0$. Hence, our goal is to prove the existence of an integral manifold for (3.1) with the representation

$$u_2 = \eta^*(u_1, t, \varepsilon) := \varepsilon\varphi(u_1, t) + O(\varepsilon^2) \quad \text{for} \quad 0 < \varepsilon \le \varepsilon^*,$$

where η^* depends continuously on its variables. We are especially interested in estimating ε^*. The underlying idea of the corresponding proof is to find the function η^* as fixed point of an appropriate operator in some complete metric space. To this end we introduce the function space $C(d, l)$, where d and l are positive constants, which consists of all functions η mapping $D := R^m \times R \times [0, \overline{\varepsilon}]$ continuously into R^k ($\overline{\varepsilon}$ is some positive number) and having the properties

$$|\eta(u_1, t, \varepsilon)| \le d \qquad \forall (u_1, t, \varepsilon) \in D, \tag{3.5}$$

$$|\eta(u_1, t, \varepsilon) - \eta(\tilde{u}_1, t, \varepsilon)| \le l\ |u_1 - \tilde{u}_1| \qquad \forall (u_1, t, \varepsilon), (\tilde{u}_1, t, \varepsilon) \in D. \tag{3.6}$$

If we endow $C(d, l)$ with the norm

$$||\eta|| = \sup_{(u_1, t, \varepsilon) \in D} |\eta(u_1, t, \varepsilon)|, \tag{3.7}$$

we get a complete metric space.

For $\eta \in C(d,l)$ we consider the initial value problem

$$\frac{du_1}{dt} = f(u_1, \eta(u_1,t,\varepsilon),t), \quad u_1(t_0) = u_1^0, \tag{3.8}$$

where u_1^0 is any given point in R^m. From (A_1) and (A_2) it follows that $f(u_1,\eta(u_1,t,\varepsilon),t)$ is continuous and uniformly bounded. Moreover, we have

$$|f(u_1,\eta(u_1,t,\varepsilon),t) - f(\tilde{u}_1,\eta(\tilde{u}_1,t,\varepsilon),t)| \le (c_{41}+c_{42}l)|u_1-\tilde{u}_1| \ \forall\ (u_1,t,\varepsilon),(\tilde{u}_1,t,\varepsilon) \in D. \tag{3.9}$$

Thus, (3.8) has a unique solution $u_1 = \varphi^\eta(t,\varepsilon,u_1^0)$ defined for $t \in R$ and satisfying $\varphi^\eta(t_0,\varepsilon,u_1^0) = u_1^0$. Substituting $\varphi^\eta(t,\varepsilon,u_1^0)$ into the second equation of (3.1) we get

$$\varepsilon\ \frac{du_2}{dt} = Bu_2 + \varepsilon g(\varphi^\eta(t,\varepsilon,u_1^0),u_2,t). \tag{3.10}$$

In the same way as above we can conclude that under our assumptions the Cauchy problem to (3.10) has a unique global solution.
Let $X(t,\tau,\varepsilon)$ be the fundamental matrix of the linear system

$$\varepsilon\ \frac{du_2}{dt} = Bu_2$$

satisfying $X(\tau,\tau,\varepsilon) = I$ that is

$$X(t,\tau,\varepsilon) = \exp\Big(B\frac{t-\tau}{\varepsilon}\Big).$$

Let $|.|$ be the matrix norm induced by the Euclidean vector norm that is $|A| = \sqrt{\varrho(A^TA)}$ where ϱ denotes the spectral radius.
According to assumption (A_3) there is a constant $c \ge 1$ such that (see, e.g., Brauer and Nohel [22])

$$|X(t,\tau,\varepsilon)| \le c\ \exp\Big(-\frac{\gamma(t-\tau)}{\varepsilon}\Big) \quad \text{for} \quad t \ge \tau \quad \text{and} \quad \varepsilon > 0. \tag{3.11}$$

If we assume that $u_2 = \eta^*(u_1,t,\varepsilon)$ with $\eta^* \in C(d,l)$ is an integral manifold $\mathcal{M}_\varepsilon^{d,l}$ of (3.1) then $\eta^*(\varphi^{\eta^*}(t,\varepsilon,u_1^0),t,\varepsilon)$ is a solution of (3.10) which is uniformly bounded. Under our assumptions it is easy to prove that a global solution of (3.10) which is uniformly bounded satisfies the integral equation

$$u_2(t,\varepsilon,u_1^0) = \int_{-\infty}^t X(t,\tau,\varepsilon)g(\varphi^\eta(\tau,\varepsilon,u_1^0),u_2(\tau,\varepsilon,u_1^0),\tau)d\tau. \tag{3.12}$$

Thus, $\eta^*(\varphi^{\eta^*}(t,\varepsilon,u_1^0),t,\varepsilon)$ satisfies (3.12). Therefore, we introduce the operator $\mathcal{T}$ defined on $C(d,l)$ by

$$(\mathcal{T}\eta)(u_1^0,t,\varepsilon) := \int_{-\infty}^t X(t,\tau,\varepsilon)g(\varphi^\eta(\tau,\varepsilon,u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon),\tau)d\tau. \tag{3.13}$$

Lemma 3.1 *Let d and l be given positive numbers. Under the assumptions $(A_1)-(A_3)$ and under the additional conditions*

$$\begin{aligned} \frac{\varepsilon c c_2}{\gamma} &\le d, && (3.14)\\ \frac{\varepsilon c(c_{51}+c_{52}l)}{\gamma-\varepsilon(c_{41}+c_{42}l)} &\le l, && (3.15)\\ \varepsilon(c_{41}+c_{42}l) &< \gamma && (3.16) \end{aligned}$$

the operator $\mathcal{T}$ maps the complete metric space $C(d,l)$ into itself.

Proof. Under our assumptions it is easy to show that $\mathcal{T}\eta$ is continuous for $\eta \in C(d,l)$. Next, we prove that $\mathcal{T}$ is uniformly bounded. From (3.13), (3.11), and (3.2) we get

$$|(\mathcal{T}\eta)(u_1^0,t,\varepsilon)| \le \int_{-\infty}^{t} c e^{-\gamma(t-\tau)/\varepsilon} c_2 d\tau = \frac{c c_2 \varepsilon}{\gamma}.$$

Now we show that $(\mathcal{T}\eta)(u_1^0,t,\varepsilon)$ is lipschitzian in u_1^0. From (3.8) it follows that

$$\begin{aligned} \varphi^\eta(s,\varepsilon,u_1^0) &= u_1^0 + \int_{t_0}^{s} f(\varphi^\eta(\sigma,\varepsilon,u_1^0),\eta(\varphi^\eta(\sigma,\varepsilon,u_1^0),\sigma,\varepsilon),\sigma)d\sigma,\\ \varphi^\eta(s,\varepsilon,\bar{u}_1^0) &= \bar{u}_1^0 + \int_{t_0}^{s} f(\varphi^\eta(\sigma,\varepsilon,\bar{u}_1^0),\eta(\varphi^\eta(\sigma,\varepsilon,\bar{u}_1^0),\sigma,\varepsilon),\sigma)d\sigma. \end{aligned} \quad (3.17)$$

Using (3.3), (3.6), (3.9) we have

$$\begin{aligned} |\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^\eta(s,\varepsilon,\bar{u}_1^0)| &\le |u_1^0-\bar{u}_1^0|\\ &\quad + \int_{t_0}^{s}(c_{41}+c_{42}l)|\varphi^\eta(\sigma,\varepsilon,u_1^0)-\varphi^\eta(\sigma,\varepsilon,\bar{u}_1^0)|d\sigma. \end{aligned}$$

By means of Gronwall's inequality (Lemma 2.1) we obtain for $s \ge t_0$

$$|\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^\eta(s,\varepsilon,\bar{u}_1^0)| \le |u_1^0-\bar{u}_1^0| e^{(c_{41}+c_{42}l)(s-t_0)}. \quad (3.18)$$

In case $s \le t_0$ we get from (3.17)

$$\begin{aligned} |\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^\eta(s,\varepsilon,\bar{u}_1^0)| &\le |u_1^0-\bar{u}_1^0|\\ &\quad + \int_{s}^{t_0}(c_{41}+c_{42}l)|\varphi^\eta(\sigma,\varepsilon,u_1^0)-\varphi^\eta(\sigma,\varepsilon,\bar{u}_1^0)|d\sigma. \end{aligned}$$

According to (2.3) (Lemma 2.2) we have

$$|\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^\eta(s,\varepsilon,\bar{u}_1^0)| \le |u_1^0-\bar{u}_1^0| e^{(c_{41}+c_{42}l)(t_0-s)}.$$

From (3.13), (3.11), (3.4), (3.6), (3.14), (3.16) and (3.18) with $s=\tau, t_0=t$ we obtain

$$\begin{aligned} &|(\mathcal{T}\eta)(u_1^0,t,\varepsilon)-(\mathcal{T}\eta)(\bar{u}_1^0,t,\varepsilon)|\\ \le\ & \int_{-\infty}^{t} c\ e^{-\gamma(t-\tau)/\varepsilon}|g(\varphi^\eta(\tau,\varepsilon,u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon),\tau)\\ & -g(\varphi^\eta(\tau,\varepsilon,\bar{u}_1^0),\eta(\varphi^\eta(\tau,\varepsilon,\bar{u}_1^0),\tau,\varepsilon),\tau)|d\tau\\ \le\ & c(c_{51}+c_{52}l)\int_{-\infty}^{t}|\varphi^\eta(\tau,\varepsilon,u_1^0)-\varphi^\eta(\tau,\varepsilon,\bar{u}_1^0)|e^{-\gamma(t-\tau)/\varepsilon}d\tau\\ \le\ & c(c_{51}+c_{52}l)|u_1^0-\bar{u}_1^0|\int_{-\infty}^{t} e^{-(\gamma-\varepsilon(c_{41}+c_{42}l))(t-\tau)/\varepsilon}d\tau = \frac{c\varepsilon(c_{51}+c_{52}l)}{\gamma-\varepsilon(c_{41}+c_{42}l)}|u_1^0-\bar{u}_1^0|. \end{aligned}$$

Hence, under the assumption of Lemma 3.1 the operator $\mathcal{T}$ maps $C(d,l)$ into itself.

Lemma 3.2 *Under the assumptions of Lemma* 3.1 *the mapping* $\mathcal{T} : C(d,l) \to C(d,l)$ *is lipschitzian in* η.

Proof. From (3.13), (3.11), (3.6) and (3.4) we get

$$\begin{aligned}
& |(\mathcal{T}\eta)(u_1^0,t,\varepsilon) - (\mathcal{T}\bar\eta)(u_1^0,t,\varepsilon)| \\
\le\ & \int_{-\infty}^{t} c\, e^{-\gamma(t-\tau)/\varepsilon} |g(\varphi^\eta(\tau,\varepsilon,u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon),\tau) \\
& -g(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\bar\eta(\varphi^{\bar\eta}(t,\varepsilon,u_1^0),\tau,\varepsilon),\tau)|d\tau \\
\le\ & c\int_{-\infty}^{t} e^{-\gamma(t-\tau)/\varepsilon}\Big(c_{51}|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)| \\
& +c_{52}(|\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon) - \eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon)| \\
& +|\eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon) - \bar\eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon)|\Big)d\tau \\
\le\ & c(c_{51}+c_{52}l)\int_{-\infty}^{t} e^{-\gamma(t-\tau)/\varepsilon}|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)|d\tau \\
& +\frac{c\varepsilon c_{52}}{\gamma}||\eta-\bar\eta||.
\end{aligned} \tag{3.19}$$

From (3.17), (3.3), and (3.7) it follows

$$\begin{aligned}
& |\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)| \\
\le\ & \int_{\tau}^{t} |f(\varphi^\eta(s,\varepsilon,u_1^0),\eta(\varphi^\eta(s,\varepsilon,u_1^0),s,\varepsilon),s) - f(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),\bar\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon),s)|ds \\
\le\ & \int_{\tau}^{t} \Big(c_{41}|\varphi^\eta(s,\varepsilon,u_1^0) - \varphi^{\bar\eta}(s,\varepsilon,u_1^0)| + c_{42}(|\eta(\varphi^\eta(s,\varepsilon,u_1^0),s,\varepsilon) - \eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon)| \\
& +|\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon) - \bar\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon)|\Big)ds \\
\le\ & \int_{\tau}^{t} \Big((c_{41}+c_{42}l)|\varphi^\eta(s,\varepsilon,u_1^0) - \varphi^{\bar\eta}(s,\varepsilon,u_1^0)|\Big)ds + c_{42}||\eta-\bar\eta||(t-\tau).
\end{aligned}$$

According to Lemma 2.2 we have

$$|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)| \le \frac{c_{42}||\eta-\bar\eta||}{c_{41}+c_{42}l}\Big(\ e^{(c_{41}+lc_{42})(t-\tau)} - 1\Big). \tag{3.20}$$

Substituting (3.20) into (3.19) and taking into account (3.16) we get

$$\begin{aligned}
& |(\mathcal{T}\eta)(u_1^0,t,\varepsilon) - (\mathcal{T}\bar\eta)(u_1^0,t,\varepsilon)| \\
\le\ & \frac{c(c_{51}+lc_{52})}{c_{41}+lc_{42}}\ c_{42}||\eta-\bar\eta||\int_{-\infty}^{t} e^{-\gamma(t-\tau)/\varepsilon}(e^{(c_{41}+lc_{42})(t-\tau)} - 1)d\tau + \frac{c\varepsilon c_{52}}{\gamma}||\eta-\bar\eta|| \\
=\ & \Big(\frac{\varepsilon^2 c(c_{51}+lc_{52})c_{42}}{\gamma(\gamma-\varepsilon(c_{41}+lc_{42}))} + \frac{c\varepsilon c_{52}}{\gamma}\Big)\ ||\eta-\bar\eta|| = \frac{c\varepsilon}{\gamma}\Big(\frac{\varepsilon(c_{51}+lc_{52})c_{42}}{\gamma-\varepsilon(c_{41}+c_{42}l)} + c_{52}\Big)||\eta-\bar\eta||.
\end{aligned}$$

From Lemma 3.1 and Lemma 3.2, by applying Banach's fixed point theorem, we obtain the result:

Lemma 3.3 *Under the assumptions of Lemma* 3.1 *and under the additional condition*

$$\frac{c\varepsilon}{\gamma}\left(\frac{\varepsilon(c_{51}+lc_{52})c_{42}}{\gamma-\varepsilon(c_{41}+c_{42}l)}+c_{52}\right)\leq q<1 \tag{3.21}$$

the operator $\mathcal{T}$ *has a unique fixed point* η^* *in* $C(d,l)$.
Since it can be easily checked that $u_2=\eta^*(u_1,t,\varepsilon)$ represents an integral manifold of (3.1), we obtain from Lemma 3.3:

Theorem 3.1 *Under the assumptions of Lemma* 3.1 *and under the additional condition* (3.21) *the singularly perturbed system* (3.1) *has an integral manifold* $\mathcal{M}_\varepsilon^{d,l}:=\{(u_1,u_2)\in R^{m+k}:u_2=\eta^*(u_1,t,\varepsilon)\}$ *where* η^* *belongs to the class* $C(d,l)$.

Remark 3.2 *It is obvious that the inequalities (3.14), (3.15), (3.16), and (3.21) are satisfied for sufficiently small* ε. *Hence, Theorem 3.1 can be formulated as*

Theorem 3.3 *Under the assumptions* $(A_1)-(A_3)$ *and for sufficiently small* ε *the singularly perturbed system* (3.1) *has an integral manifold* $\mathcal{M}_\varepsilon^{d,l}:=\{(u_1,u_2)\in R^{m+k}:u_2=\eta^*(u_1,t,\varepsilon)\}$ *where* η^* *belongs to the class* $C(d,l)$.

For given d and l the inequalities (3.14), (3.15), (3.16), and (3.21) determine a maximal positive number $\varepsilon^*(d,l)$ such that (3.1) has an integral manifold $\mathcal{M}_\varepsilon^{d,l}$ for $0\leq\varepsilon<\varepsilon^*$. With respect to applications we want to maximize ε^*. Since we are more interested to prescribe a small neighborhood of the origin (measured by d) than a small Lipschitz constant, we will use l to maximize ε^*.
If $c_{41}=c_{42}=c_{51}=c_{52}=0$ then the inequalities (3.15), (3.16) and (3.21) are satisfied trivially. Now we assume that at least one of these constants is positive.
From (3.16) and (3.15) we get the inequalities

$$\begin{aligned}\varepsilon &< \frac{\gamma}{c_{41}+c_{42}l}=:\varepsilon_1(l),\\ \varepsilon &\leq \frac{l\gamma}{c(c_{51}+c_{52}l)+l(c_{41}+c_{42}l)}=:\varepsilon_2(l).\end{aligned}$$

It is obvious that

$$\varepsilon_1(l)\geq\varepsilon_2(l)\quad\text{for}\quad l\geq 0.$$

Under the condition (3.15), the inequality (3.21) is equivalent to

$$\varepsilon^2c(c_{51}c_{42}-c_{52}c_{41})+\varepsilon\,\gamma(c_{52}c+c_{41}+c_{42}l)<\gamma^2. \tag{3.22}$$

Let us introduce the notation

$$\kappa:=c(c_{42}c_{51}-c_{41}c_{52}),\quad \mu:=cc_{52}+c_{41}+c_{42}l.$$

In case $\kappa=0$, (3.22) reads

$$\varepsilon<\frac{\gamma}{c_{52}c+c_{41}+c_{42}l}:=\varepsilon_3(l).$$

It is easy to verify that $\varepsilon_2(l) \leq \varepsilon_3(l)$ for all $l \geq 0$.
The case $\kappa < 0$ can be reduced to the case $\kappa = 0$. Now we assume $\kappa > 0$. In that case, (3.22) is equivalent to

$$\varepsilon^2 + \varepsilon\frac{\gamma\mu}{\kappa} < \frac{\gamma^2}{\kappa}. \tag{3.23}$$

It is obvious that (3.23) is satisfied for

$$\varepsilon < \frac{\gamma}{2\kappa}\Big(-\mu + \sqrt{\mu^2 + 4\kappa}\Big) = \frac{2\gamma}{\sqrt{\mu^2 + 4\kappa} + \mu} =: \varepsilon_4(l).$$

Proving that $\varepsilon_2(l) \leq \varepsilon_4(l)$ for $l \geq 0$ is equivalent to establishing that

$$\frac{l}{cc_{51} + l\mu} \leq \frac{2}{\sqrt{\mu^2 + 4\kappa} + \mu}.$$

This inequality holds if we have

$$l^2\kappa \leq c^2c_{51}^2 + cc_{51}l\mu. \tag{3.24}$$

The validity of (3.24) follows from the obvious inequality

$$l\kappa \leq cc_{51}\mu.$$

Consequently, to maximize ε^* as a function of l we have to look for the maximum of $\varepsilon_2(l)$. It is easy to verify that $\varepsilon_2(l)$ takes its maximum

$$\gamma/(cc_{52} + 2\sqrt{cc_{51}c_{42}} + c_{41})$$

at

$$l = l^* := \frac{\sqrt{cc_{42}c_{51}}}{c_{42}}.$$

Thus, we have:

Lemma 3.4 *Under the assumptions*

$$c_{51} > 0, \quad c_{42} > 0,$$

ε^* takes its maximum for $l = l^*$.

4 Local state space reduction

Let us return to our original n-dimensional system

$$\frac{dz}{dt} = h(z,t) \qquad (z,t) \in R^n \times R \tag{4.1}$$

and assume that h is twice continuously differentiable with respect to z and t. The goal of our investigations is to derive conditions which ensure that we can approximate a solution of (4.1) in some regions of the (z,t)-space by a solution of a system of differential equations whose

dimension of the state space is less than n. To justify such a reduction we will exploit the existence of an attracting locally invariant manifold (a.l.i.m.) of (4.1) near the point (z_0, t_0).

For these purposes we transform system (4.1) into a form to which we can apply Theorem 3.1. Let (z_0, t_0) be a given point. We use the upper index ^{0} in order to indicate that we consider some expression at the point (z_0, t_0). Under our differentiability assumptions, (4.1) is equivalent to the system

$$\frac{dz}{dt} = h^0 + J^0(z - z_0) + \tilde{h}(z, t, z_0, t_0) \tag{4.2}$$

where

$$\tilde{h}(z, t, z_0, t_0) = h(z, t) - h^0 - J^0(z - z_0), \quad J^0 = h_z(z_0, t_0).$$

Near (z_0, t_0) we have

$$\tilde{h}(z, t, z_0, t_0) = O(|z - z_0|^2 + |t - t_0|).$$

Now we compute the spectrum σ^0 of J^0 and decompose it into the disjoint sets $\sigma^0_{-\nu}$ and σ^0_r where the real parts of all eigenvalues of $\sigma^0_{-\nu}$ are less than $-\nu, \nu > 0$. From the method of block diagonalization it follows that there is a regular matrix T such that

$$T^{-1} J^0 T =: S^0 = \text{ diag } (S^0_{11}, S^0_{22}), \tag{4.3}$$

where S^0_{11} and S^0_{22} are upper triangular matrices with possible non-vanishing entries on the first sub-diagonal related to complex conjugate eigenvalues and such that $\sigma(S^0_{11}) = \sigma^0_r,\ \sigma(S^0_{22}) = \sigma^0_{-\nu}$. Applying the coordinate transformation $z = z_0 + Tu$ we get from (4.2)

$$\frac{du}{dt} = T^{-1} h^0 + S^0 u + T^{-1} \tilde{h}(z_0 + Tu, t, z_0, t_0). \tag{4.4}$$

Taking into account the block diagonal structure (4.3) we may represent (4.4) in the form

$$\begin{aligned} \frac{du_1}{dt} &= \hat{h}^0_1 + S^0_{11} u_1 + \bar{h}_1(u, t, z_0, t_0), \\ \frac{du_2}{dt} &= \hat{h}^0_2 + S^0_{22} u_2 + \bar{h}_2(u, t, z_0, t_0). \end{aligned} \tag{4.5}$$

Now we multiply the second equation with ε_ν, $\varepsilon_\nu := \nu^{-1}$, and denote by $\overline{S}^0_{22}$ the matrix defined by $\overline{S}^0_{22} := \varepsilon_\nu S^0_{22}$. Then (4.5) reads

$$\begin{aligned} \frac{du_1}{dt} &= \hat{h}^0_1 + S^0_{11} u_1 + \bar{h}_1(u, t, z_0, t_0), \\ \varepsilon_\nu \frac{du_2}{dt} &= \varepsilon_\nu \hat{h}^0_2 + \overline{S}^0_{22} u_2 + \varepsilon_\nu \bar{h}_2(u, t, z_0, t_0), \end{aligned}$$

where all eigenvalues of $\overline{S}^0_{22}$ have real parts less than -1. In what follows we consider the singularly perturbed system

$$\begin{aligned} \frac{du_1}{dt} &= S_{11}^0 u_1 + \hat{h}_1^0 + \bar{h}_1(u,t,z_0,t_0), \\ \varepsilon\,\frac{du_2}{dt} &= \overline{S}_{22}^0 u_2 + \varepsilon\hat{h}_2^0 + \varepsilon\bar{h}_2(u,t,z_0,t_0) \end{aligned} \tag{4.6}$$

for $0 \le \varepsilon \le \varepsilon_\nu$ which has the same structure as system (3.1) with

$$\begin{aligned} f(u_1,u_2,t) &= S_{11}^0 u_1 + \hat{h}_1^0 + \bar{h}_1(u_1,u_2,t,z_0,t_0)), \\ g(u_1,u_2,t) &= \hat{h}_2^0 + \bar{h}_2(u_1,u_2,t,z_0,t_0). \end{aligned}$$

For $\varepsilon = 0$, (4.6) has the invariant manifold $u_2 \equiv 0$. If we are able to prove that (4.6) has an a.l.i.m. $u_2 = \eta^*(u_1,t,\varepsilon) = \varepsilon\varphi(u_1,t) + O(\varepsilon^2)$ for $0 < \varepsilon \le \varepsilon_\nu$ passing a d-neighborhood of $(u = 0, t = t_0)$ then we can conclude that also (4.1) has a locally invariant exponentially attracting manifold near (z_0,t_0). If additionally (z_0,t_0) lies in the region of attraction of this invariant manifold and d is small then we can approximate the orbit of (4.1) through (z_0,t_0) by an orbit of the reduced differential system

$$\frac{du_1}{dt} = S_{11}^0 u_1 + \hat{h}_1^0 + \bar{h}_1(u_1,\varepsilon\varphi(u_1,t),t,z_0,t_0). \tag{4.7}$$

Now we describe the procedure to finding out the essential variables in system (4.1) near (z_0,t_0) by means of Theorem 3.1 which is equivalent to a local reduction of the state space.

S1. We compute the spectrum σ^0 of J^0. If σ^0 has no eigenvalue with negative real part, then we replace (z_0,t_0) by another point (which we get, for example, by numerical integration starting at (z_0,t_0)). In case we do not find any point (z_0,t_0) we are not able to reduce the dimension of the phase space by this method.

S2. We assume σ^0 has eigenvalues with negative real parts $-\lambda_k < \ldots < -\lambda_1 < 0$ (It suffices to have at least one). We choose a negative number $-\nu$, the so-called splitting parameter, such that we have $-\lambda_j < -\nu < -\lambda_{j-1}$ for some j and compute the real Schur decomposition $S^0 = \operatorname{diag}(S_{11}^0, S_{22}^0)$ to the splitting parameter $-\nu$, that is

$$\begin{aligned} \text{Re } \sigma(S_{22}^0) &\le -\lambda_j \le -\nu, \\ \text{Re } \sigma(S_{11}^0) &\ge -\nu. \end{aligned}$$

In case that the eigenvalues of S_{22}^0 with the real part $-\lambda_j$ are simple, we can put $\nu = \lambda_j$ in all other cases we assume $\nu < \lambda_j$. Now we set $\varepsilon_\nu := \nu^{-1}$. Thus we have $\text{Re } \sigma(S_{22}^0) < \gamma = 1$.

S3. We transform (4.1) into the form (4.6).

S4. Let $\sum_\varrho$ be the ball in $R_{u_1}^m \times R_{u_2}^k \times R$ with radius ϱ centered at $(0,t_0)$. We choose a (small) number d (c.f. (3.5)) and derive estimates for the constants $c_1, c_2, c_{41}, c_{42}, c_{51}, c_{52}$ introduced in assumption (A_2) with respect to $\sum_d$.

S5. We compute the constant c to estimate $\left|e^{B(t-\tau)/\varepsilon}\right|$. (In the case where all eigenvalues are simple we can set $c = 1$.)

S6. We calculate l^* and check the inequalities (3.14) – (3.16) and (3.21) with $\gamma = 1, \varepsilon = \varepsilon_\nu$. If the inequalities are satisfied then we can state the existence of a local integral manifold of (1.2) in $\sum_d$ by means of Theorem 3.1 and system (4.1) can be reduced to (4.7). If the inequalities are not satisfied we go back to S2 and choose a splitting parameter ν with larger modulus, i.e., the corresponding ε_ν becomes smaller.

S7. In case we cannot further increase the modulus of ν we replace (z_0, t_0) by another point and go back to S1.

In case that d is sufficiently small we can approximate the constants $c_2, \cdots, c_{52}$ as follows

$$c_2 \approx |\hat{h}_2^0|,\ c_{41} \approx |S_{11}^0|,\ c_{42} \approx 0,\ c_{51} \approx 0,\ c_{52} \approx 0.$$

If we use these approximations we call the corresponding algorithm a simplified algorithm. In case of the simplified algorithm we have $\varepsilon_1(l) \equiv \varepsilon_2(l) \equiv \varepsilon_3(l) \equiv \varepsilon_4(l) \equiv |S_{11}^0|^{-1}$. Thus, the Lipschitz constant l has no influence on ε^*. To prove that (4.6) has an invariant manifold for $\varepsilon = \varepsilon_\nu$ we have to verify the inequalities (3.14) – (3.16) and (3.21) which are equivalent under our assumptions to

$$\frac{|S_{11}^0|}{\nu} < 1, \quad \frac{c|\hat{h}_2^0|}{\nu} < d. \tag{4.8}$$

We note that in the case when all eigenvalues of J^0 have negative real parts then the first of the inequalities (4.8) is always satisfied.

5 Examples

The following examples of chemical reactions will be used to illustrate our simplified algorithm to determine fast and slow variables by localizing an invariant manifold, and therefore to give a local reduction of the dimension of the state space. All necessary calculations were performed by MAPLE and MATLAB.

5.1 Example by Duchêne/Rouchon

The following simple reaction scheme has been considered in Duchêne and Ruchon [17]:

$$X_1 \xrightarrow{k_1} X_2, \quad X_2 \xrightarrow{k_2} X_1, \quad X_1 + X_2 \xrightarrow{\delta k_0} X_2 + X_3,$$

where X_1, X_2, X_3 are chemical species, and k_1, k_2, and δk_0 are reaction rate constants. The small parameter $\delta > 0$ is used to indicate that the third reaction is slow in comparison with the other two reactions. This reaction scheme can be described by the system of ordinary differential equations

$$\begin{aligned}
\frac{dx_1}{dt} &= -k_1 x_1 + k_2 x_2 - \delta k_0 x_1 x_2, \\
\frac{dx_2}{dt} &= k_1 x_1 - k_2 x_2, \\
\frac{dx_3}{dt} &= \delta k_0 x_1 x_2,
\end{aligned}$$

where x_i is the concentration of $X_i, i = 1, 2, 3$. It is obvious that the third equation is a linear combination of the first and the second one so that we can restrict ourselves to the system

$$\begin{aligned} \frac{dx_1}{dt} &= -k_1 x_1 + k_2 x_2 - \delta k_0 x_1 x_2, \\ \frac{dx_2}{dt} &= k_1 x_1 - k_2 x_2. \end{aligned} \tag{5.1}$$

Before we apply our (simplified) algorithm to (5.1) we will prove the existence of an invariant manifold for (5.1) and derive an asymptotic approximation of it. By this way we able to study the effectivity of the proposed procedure.
By means of the coordinate transformation $\xi = x_1 + x_2, \quad x_2 = x_2$ we get from (5.1)

$$\begin{aligned} \frac{d\xi}{dt} &= -\delta\, k_0\, (\xi - x_2)\, x_2, \\ \frac{dx_2}{dt} &= k_1\, (\xi - x_2) - k_2\, x_2. \end{aligned} \tag{5.2}$$

By rescaling the time t, $t = \delta^{-1}\, \tau$, and introducing the notation $\xi(\delta^{-1}\, \tau) = y_1(\tau),\ x_2(\delta^{-1}\, \tau) = y_2(\tau)$ we obtain from (5.2)

$$\begin{aligned} \frac{dy_1}{d\tau} &= -k_0\, y_1\, y_2 + k_0\, y_2^2, \\ \delta\, \frac{dy_2}{d\tau} &= k_1\, y_1 - (k_1 + k_2)\, y_2 \end{aligned} \tag{5.3}$$

which represents a singularly perturbed system. The corresponding degenerate equation

$$0 = k_1\, y_1 - (k_1 + k_2)\, y_2 := g(y_1, y_2)$$

has the unique solution

$$y_2 = h_0(y_1) := \frac{k_1}{k_1 + k_2}\, y_1,$$

moreover the corresponding inequality holds

$$J(y_1, h_0(y_1)) := \frac{\partial g}{\partial y_2}_{|y_2 = h_0(y_1)} = -(k_1 + k_2) < 0.$$

By the transformation

$$y_2 = w_2 + \frac{k_1}{k_1 + k_2}\, y_1,$$

we obtain from (5.3) the system

$$\begin{aligned} \frac{dy_1}{d\tau} &= -\frac{k_0 k_1 k_2}{(k_1 + k_2)^2} y_1^2 + \frac{k_0 (k_1 - k_2)}{k_1 + k_2} y_1 w_2 + k_0 w_2^2, \\ \delta\, \frac{dw_2}{d\tau} &= -(k_1 + k_2) w_2 - \frac{\delta k_1}{k_1 + k_2} \Big\{ -\frac{k_0 k_1 k_2}{(k_1 + k_2)^2} y_1^2 + \frac{k_0 (k_1 - k_2)}{k_1 + k_2} y_1 w_2 + k_0 w_2^2 \Big\} \end{aligned} \tag{5.4}$$

which has the form (3.1). It is easy to verify that in a compact region of the phase plane all conditions of Theorem 3.1 are satisfied for sufficiently small δ. Thus, (5.4) has an invariant manifold of $\mathcal{M}_\delta$ of the form

$$w_2 = \delta\varphi_1(y_1) + O(\delta^2).$$

A straightforward computation yields

$$\varphi_1(y_1) := \frac{k_0 k_1^2 k_2}{(k_1+k_2)^4} y_1^2,$$

hence we have

$$w_2 = \delta\frac{k_0 k_1^2 k_2}{(k_1+k_2)^4} y_1^2 + O(\delta^2).$$

In the original coordinates $\mathcal{M}_\delta$ has the implicit representation

$$x_2 = \frac{k_1}{k_1+k_2}(x_1+x_2)\Big(1+\delta\frac{k_0 k_1 k_2}{(k_1+k_2)^3}(x_1+x_2) + O(\delta^2)\Big). \tag{5.5}$$

In what follows we apply the simplified algorithm to system (5.1) in order to decide whether near a given point x^0 the dimension of the phase space can be reduced. In the sequel we fix the parameters as

$$k_0 = 10, \qquad k_1 = 2, \qquad k_2 = 3, \qquad \delta = 0.01,$$

so that (5.1) reads

$$\begin{aligned} \frac{dx_1}{dt} &= -2x_1 + 3x_2 - 0.1x_1x_2, \\ \frac{dx_2}{dt} &= 2x_1 - 3x_2. \end{aligned}$$

Table 1 contains the sample of four points (x_1^0, x_2^0) to be considered.

	Io	IIo	IIIo	IVo
x_1^0	2.0000	0.5000	3.0000	0.0000
x_2^0	5.0000	2.0000	0.5000	0.0000

Table 1. Coordinates of the first sample.

Now we use our simplified approach to check whether these points are near an exponentially attracting integral manifold of system (5.1) and thus, whether the dimension of the phase space may be reduced in some neighborhood of these points.
First we apply the coordinate transformation described in section 4 to (5.1) with respect to each initial point (cases $I_0 - IV_0$). In case Io we obtain

$$\begin{aligned} \frac{du_1}{dt} &= -1.1889 - 0.3704u_1 - 0.0335u_1^2 - 0.0073u_1u_2 + 0.0356u_2^2 \\ \frac{du_2}{dt} &= -14.8091 - 5.1296u_2 + 0.0292u_1^2 + 0.0064u_1u_2 - 0.0311u_2^2, \end{aligned}$$

Analogous systems we get in the other cases.
As neighborhood Σ_d of $u_1 = u_2 = 0$ we choose a disc with radius $d = 0.3$ that is,
$\Sigma_{0.3} := \{u \in R^2 : |u| \leq 0.3\}$. From $x - x^0 = Tu$ we get

$$|x - x^0| \leq |T|\, d := r_0.$$

Since the eigenvalues are simple, we set $\varepsilon_\nu^{-1} = \nu = |\lambda_2|$, so that we have $\gamma = 1$. Obviously, $c = 1$ holds, and we obtain the results represented in Table 2.

	Io	IIo	IIIo	IVo
λ_1	-0.3704	-0.1383	-0.1532	0
$\lambda_2 = -\nu$	-5.1296	-5.0617	-4.8968	-5
$\lvert S_{11}^0\rvert/\nu$	0.0722	0.0273	0.0313	0
$\lvert\hat{h}_2^0\rvert/\nu$	2.8870	1.3642	1.2978	0
d	0.3	0.3	0.3	0.3
$\lvert T\rvert$	1.0876	1.1011	1.0765	1.1049
$\lvert T\rvert\, d = r_0$	0.3263	0.3303	0.3229	0.3315

Table 2. Characteristic data determined by the simplified algorithm.

Since all eigenvalues are negative the condition $|S_{11}^0|/\nu < 1$ is satisfied in all cases, but the condition $|\hat{h}_2^0|/\nu < d = 0.3$ does not hold in the cases Io-IIIo.

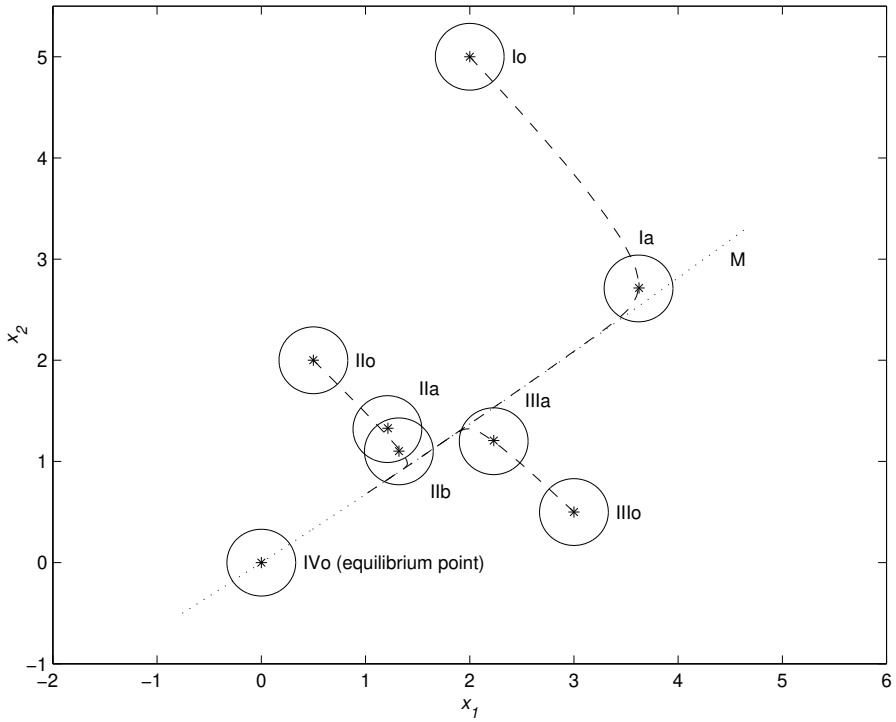

Figure 1. Invariant manifold M and location of the selected points.

Figure 1 shows the invariant manifold M (dotted line) and the solutions of (5.1) for the start points I_0 - IV_0. It can be seen that corresponding trajectories tend to the curve M which is the zeroth-order approximation of the attracting invariant manifold $\mathcal{M}_\delta$, and that $u_1 = u_2 = 0$ is located on M. The balls centered at the corresponding points have the radii $r_0 = |T|\, d$. We should note that T, and hence r_0, depends on the given point. If the inequalities (4.8) are satisfied for some points, then the corresponding balls contain an a.l.i.m. of (5.1). It is obvious that in the cases Io-IIIo the initial points have a distance to M which is larger than r_0.
Now we compute the trajectories with the initial points Io - IIIo for some time steps and get the new points described in Table 3.

	Ia	IIa	IIb	IIIa
x_1^0	3.6247	1.2147	1.3204	2.2301
x_2^0	2.7154	1.3286	1.1027	1.2067

Table 3. Coordinates of the second sample.

If we repeat the calculations above we obtain the following results represented in Table 4.

	Ia	IIa	IIb	IIIa
λ_1	-0.3084	-0.1262	-0.1182	-0.1613
$\lambda_2 = -\nu$	-4.9616	-5.0079	-4.9916	-4.9631
$\lvert S_{11}^0 \rvert/\nu$	0.0622	0.0252	0.0237	0.0325
$\lvert \hat{h}_2^0 \rvert/\nu$	0.1369	0.3995	0.1788	0.2555
d	0.3	0.3	0.3	0.3
$\lvert T \rvert$	1.0711	1.0943	1.0933	1.0846
$\lvert T \rvert\, d = r_0$	0.3213	0.3283	0.3279	0.3254

Table 4. Characteristic data determined by the simplified algorithm.

We see that the inequality $|\hat{h}_2^0|/\nu < 0.3$ is not satisfied only in the case IIa. Moreover, Figure 1 shows that the computed points Ia, IIb, IIIa have a distance to M which is smaller than r_0 that is, the corresponding balls contain an a.l.i.m., but in the case IIa this distance is larger than r_0. Thus, the cases IIa and IIb show that the method works very exactly. Consequently, in the cases Ia, IIb and IIIa the phase space can be reduced.

5.2 Oregonator

The following differential system describes the basic mechanism of the oxidation of malonic acid in an acid medium by bromate ions catalyzed by cerium, of the so-called Belousov-Zhabotinskii reaction. It represents the Field - Noyes model also known as Oregonator. We consider it in the form (see e.g., Murray [18])

$$\begin{aligned} \delta_1 \frac{dx_1}{dt} &= x_1 + q\, x_2 - x_1\, x_2 - x_1^2, \\ \frac{dx_2}{dt} &= \delta_2^{-1}(-q\, x_2 + 2\, f\, x_3 - x_1\, x_2), \\ \frac{dx_3}{dt} &= x_1 - x_3, \end{aligned} \tag{5.6}$$

where δ_1, δ_2, and q are small positive constants, f is assumed to be near 0.5. System (5.6) has two biochemically relevant equilibrium points $P^u = (0,0,0)$, $P^s = (x_1^s, x_2^s, x_3^s)$ where

$$x_1^s = 1/2(1-2\,f-q) + [(1-2\,f-q)^2 + 4\,q(1+2\,f)]^{1/2}, \quad x_2^s = \frac{2\,f\,x_1^s}{q+x_1^s}, \quad x_3^s = x_1^s.$$

The equilibrium point $P^u = (0,0,0)$ is unstable, the Jacobi matrix of (5.6) at P^s has at least one eigenvalue with negative real part (see also Murray [18]). By a suitable choice of the constants δ_1, δ_2, q, the equilibrium point P^s can be made asymptotically stable. It can be shown that to given δ_2, q, f, system (5.6) has for sufficiently small δ_1 an invariant manifold $\mathcal{M}_\delta$ (see Schneider [23, 24]). In what follows we set

$$\delta_1 = 10^{-5},\ \delta_2 = 10^{-1},\ q = 10^{-4},\ f = 0.5.$$

Then, the zeroth order approximation of $\mathcal{M}_\delta$ can be obtained by setting $\delta_1 = 0$ in the first equation of (5.6)

$$x_1 + 10^{-4}x_2 - x_1x_2 - x_1^2 = 0 \tag{5.7}$$

and solving this equation with respect to x_1. It is obvious that the branch k of the solution set of (5.7) is located in the positive orthant of the x_2, x_1 - plane and can be approximated by the straight lines $x_1 = 1 - x_2$ for $0 < x_2 \leq 1$ and by $x_1 = 0$ for $x_2 > 1$. The projection of the zeroth order approximation of $\mathcal{M}_\delta$ into the x_2, x_1-plane coincides with the curve k. Now we consider the sample of points described in Table 5,

	Io	IIo	IIIo
x_1^0	1.1000	0.3000	0.0141
x_2^0	1.2000	0.5000	0.9929
x_3^0	1.1000	0.4000	0.0141

Table 5. Coordinates of the first sample.

and ask whether near these points there is an attracting locally invariant manifold (a.l.i.m.) such that we can reduce the dimension of the phase space. There exists a coordinate transformation $x - x^0 = Tu$ such that system (5.6) takes the form (4.5). In case Io we obtain

$$\begin{aligned}
\frac{du_1}{dt} &= -2.5559u_1 + 11.1917 + 2.6319u_1^2 + 11.6813u_2^2 + 192.09u_3^2, \\
&\quad -11.4474u_1u_2 + 44.9696u_1u_3 - 97.7963u_2u_3 \\
\frac{du_2}{dt} &= -3.9455u_2 - 1.9696 - 0.6516u_1^2 - 2.1624u_2^2 - 47.5535u_3^2 \\
&\quad +2.5652u_1u_2 - 11.1326u_1u_3 + 21.9149u_2u_3 \\
\frac{du_3}{dt} &= -240005u_3 + 130897 - 17521u_1^2 + 109257u_2^2 - 1279179u_3^2 \\
&\quad +7326.14u_1u_2 - 299466u_1u_3 + 62583u_2u_3.
\end{aligned} \tag{5.8}$$

We obtain analogous systems in the other cases. Our goal is to show that near some points $u = u^0$ there is an attracting locally invariant manifold of (5.8). We note that the coefficients of

the higher order terms in (5.8) are large. In order to be able to apply our simplified algorithm we have to choose the radius d sufficiently small. In our case we set $d = 10^{-3}$. The corresponding radius in the original coordinates can then be estimated by $r_0 = |T|d$. The results of our simplified algorithm are summarized in Table 6.

	Ia	Ib	IIo	IIIo
λ_1	-2.5559	-2.5559	$+2.0016$	$+0.0345$
λ_2	-3.9455	-3.9455	$+8.9775$	$+5.3791$
λ_3	-240005	-240005	-10014	-2120
ν	$\lvert\lambda_2\rvert$	$\lvert\lambda_3\rvert$	$\lvert\lambda_3\rvert$	$\lvert\lambda_3\rvert$
$\lvert S_{11}^0\rvert/\nu$	0.6478	$1.64 \cdot 10^{-5}$	$8.9649 \cdot 10^{-4}$	$2.5368 \cdot 10^{-3}$
$\lvert\hat{h}_2^0\rvert/\nu$	33176	0.5445	0.1901	0
d	10^{-3}	10^{-3}	10^{-3}	10^{-3}
$\lvert T\rvert$	8.4057	8.4057	5.1049	2.8256
$\lvert T\rvert\, d = r_0$	0.009	0.009	0.006	0.003

Table 6. Characteristic data determined by the simplified algorithm.

Since in case Io three different negative eigenvalues exist we can use two essentially different scaling parameters ($\nu = |\lambda_2|$ in case Ia and $\nu = |\lambda_3|$ in case Ib), but the fact that the initial point in case I is far from the invariant manifold implies that no scaling is successful. The inequalities (4.8) can be verified only in case IIIo which represents a stable equilibrium point. In that case, our algorithm says that in a ball with radius 0.003 centered at the equilibrium point an a.l.i.m. of (5.6) is located. This fits into the theory that the equilibrium point is located on the invariant manifold. Now we use numerical integration to get new points in the cases Io and IIo represented in the Table 7.

	Ic	IIa
x_1^0	0.0002	0.4623
x_2^0	1.4300	0.5414
x_3^0	0.0002	0.4623

Table 7. Coordinates of the second sample.

	Ic	IIa
λ_1	-0.0020	$-0.1010 + 3.0313\,i$
λ_2	-0.9975	$-0.1010 - 3.0313\,i$
λ_3	-40040.0	-46005.4
ν	40040.0	46005.4
$\lvert S_{11}^0\rvert/\nu$	$2.4912 \cdot 10^{-5}$	$2.1959 \cdot 10^{-5}$
$\lvert\hat{h}_2^0\rvert/\nu$	$1.4975 \cdot 10^{-4}$	$1.1823 \cdot 10^{-4}$
d	10^{-3}	10^{-3}
$\lvert T\rvert$	10.1441	2.6543
$\lvert T\rvert\, d = r_0$	0.011	0.003

Table 8. Characteristic data determined by the simplified algorithm.

Table 8 contains the characteristic data determined by the simplified algorithm applied to these new points. Now, in both cases the conditions (4.8) are satisfied and we can justify the existence of an a.l.i.m. of system (5.6) in a sphere with radius 0.01 in case Ia and 0.003 in case IIa.

5.3 Simplified reaction mechanism describing dynamics of ozone in the troposphere

The following simplified reaction mechanism describing the dynamics of species in the troposphere was introduced in Kalachev and Field [20]:

$$O_3 + h\nu + (H_2O) \stackrel{k_1}{\to} 2HO^{\cdot} + (O_2), \quad HO^{\cdot} + CO + (O_2) \stackrel{k_2}{\to} HO_2^{\cdot} + (CO_2),$$

$$HO_2^{\cdot} + O_3 \stackrel{k_3}{\to} HO^{\cdot} + (2O_2), \quad NO + O_3 \stackrel{k_4}{\to} NO_2 + (O_2),$$

$$NO_2 + h\nu + (O_2) \stackrel{k_5}{\to} NO + O_3, \quad HO_2^{\cdot} + NO \stackrel{k_6}{\to} HO^{\cdot} + NO_2,$$

$$HO + NO_2 \stackrel{k_7}{\to} (HNO_3).$$

In this mechanism the concentrations of species O_2 and H_2O are assumed to be constant. Presence of $h\nu$ is some of the relations means that the corresponding reactions are photochemical. The numerical values of reaction rate constants are taken to be $k_1 = 6.9 \times 10^{-8}$, $k_5 = 3.9 \times 10^{-3}$ (s^{-1}), $k_2 = 1.9 \times 10^{-13}$, $k_3 = 1.5 \times 10^{-15}$, $k_4 = 7.9 \times 10^{-15}$, $k_6 = 9.6 \times 10^{-12}$, $k_7 = 1.3 \times 10^{-11}$ (cm^3/(molec.s)).
The emissions of CO, O_3 and NO are also taken into account. Their corresponding rates in molec./(cm^3s) are $F_{CO} = 5.0 \times 10^5$, $F_{O_3} = 6.0 \times 10^4$; F_{NO} is considered to be a parameter of order $O(10^4 - 10^5)$. In what follows, the time variable is scaled by 10^6 s.
Under condition of ideally mixed troposphere the behavior of the concentrations of the species is described by the system of ordinary differential equations

$$\begin{aligned}
\frac{dx_1}{dt} &= -k_2 x_1 x_5 + F_{CO}, \\
\frac{dx_2}{dt} &= -k_1 x_2 - k_3 x_6 x_2 - k_4 x_3 x_2 + k_5 x_4 + F_{O_3}, \\
\frac{dx_3}{dt} &= -k_4 x_3 x_2 + k_5 x_4 - k_6 x_6 x_3 + F_{NO}, \\
\frac{dx_4}{dt} &= k_4 x_3 x_2 - k_5 x_4 + k_6 x_6 x_3 - k_7 x_5 x_4, \\
\frac{dx_5}{dt} &= 2k_1 x_2 - k_2 x_5 x_1 + k_3 x_6 x_2 + k_6 x_6 x_3 - k_7 x_5 x_4, \\
\frac{dx_6}{dt} &= k_2 x_5 x_1 - k_3 x_6 x_2 - k_6 x_6 x_3.
\end{aligned} \tag{5.9}$$

Here x_1, x_2, x_3, x_4, x_5 and x_6 are the concentrations of CO, O_3, NO, NO_2, HO and HO_2, respectively. System (5.9) has been studied in Field et al. [19]. Depending on F_{NO}, different types of the long-time behavior of solutions to this system have been observed. They include (case I) transition to a stable steady state ($F_{NO} = 1.5 \times 10^4$, see Fig. 2a), (case II) a stable limit cycle ($F_{NO} = 5.0 \times 10^4$, see Fig. 2b), (case III) chaotic behavior ($F_{NO} = 7.6 \times 10^4$, see Fig. 2c).

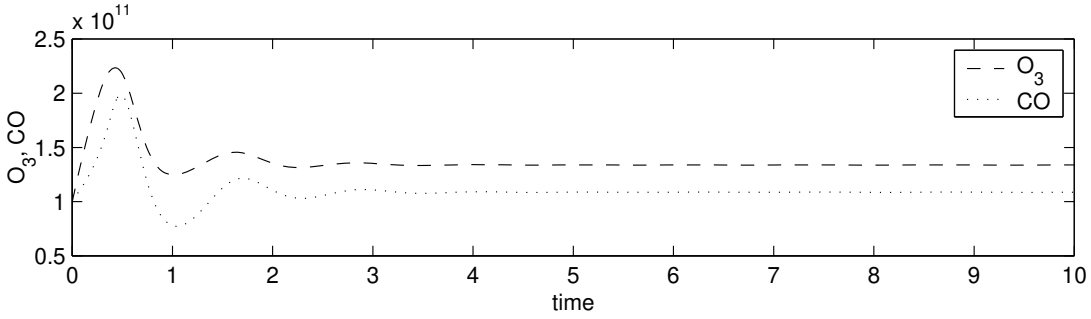

Figure 2a. Solution of (5.9) tending to an equilibrium.

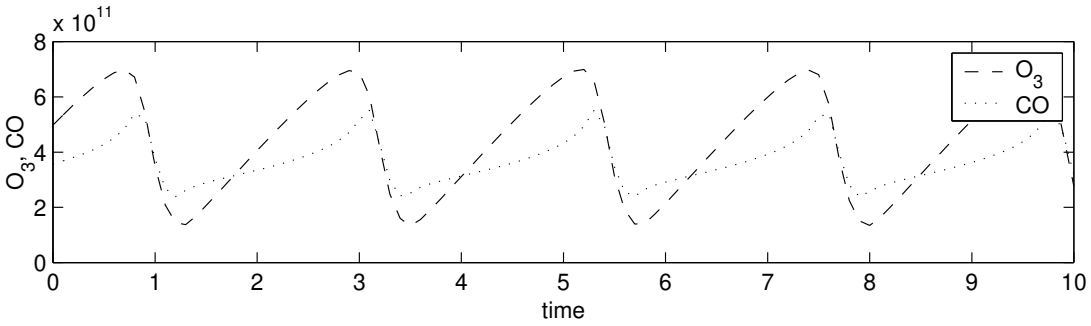

Figure 2b. Periodic solution of (5.9).

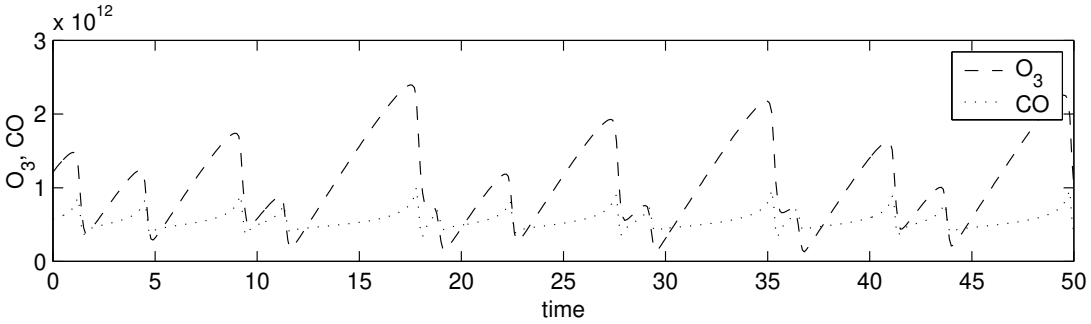

Figure 2c. Chaotic solution of (5.9).

Estimation of a number of phase variables sufficient for complete description of all the types of behavior mentioned above is an important topic actively discussed in the literature (see, e.g., Heard et al. [25], and Krol and Poppe [26]). Most authors, however, currently use heuristic methods for the analysis.

Here we apply the simplified algorithm to study the dimension of the underlying long-time dynamics of the originally six-dimensional tropospheric model. For that we choose some points which are located on or very near to the trajectories represented in the figures above. The points used in the algorithm are presented in Table 9.

	I ($\times 10^7$)	IIa ($\times 10^6$)	IIb ($\times 10^7$)	IIIa ($\times 10^5$)	IIIb ($\times 10^7$)
x_1^0	13536	507481	31361	1643120	66123
x_2^0	11051	360233	34711	5384483	58646
x_3^0	1	4009	1	1683876	2
x_4^0	6	2944	1	1837126	2
x_5^0	2	1	4	3	3
x_6^0	186	3	332	6	368

Table 9. Points chosen on the trajectories shown in Figures 2a–2c.

Chosen points are taken at different locations on various trajectories representing characteristic features of possible types of behavior of the system. Point I corresponds to a situation when the trajectory relaxes to a stable steady state. It is known that oscillatory trajectories of the tropospheric chemistry systems usually have two very distinct phases: so-called, high- and low-NOx regimes (i.e., the regimes for which the concentrations of both NO and NO_2 are high or low; see, e.g., Stewart [27]). These two regimes are characterized by domination of completely different underlying chemical processes, and that is why the question on estimation of local underlying dimensions for both cases is so very interesting. Points IIa and IIb belong to an oscillatory trajectory for high- and low-NOx subintervals within a period of an oscillation, respectively. Points IIIa and IIIb correspond to high- and low-NOx situations in the case of chaotic behavior of the system.
Same as in the previous examples, we represent the values of various parameters computed according to the simplified algorithm in Table 10. We note that in this example $c = 1$ also.

	I	IIa	IIb	IIIa	IIIb
λ_1	$-2+5i$	0.0	$-3+9i$	0.0	$-0.0+0.0i$
λ_2	$-2-5i$	0.0	$-3-9i$	0.0	$-0.0-0.0i$
λ_3	-2	-0.0	-2	-0.0	-0.0
λ_4	-306	-6870	-499	-8290	-440
λ_5	-21734	-9010	-58194	-59310	-43750
λ_6	-27545	-164660	-61922	-654170	-129240
ν	306	6870	499	8290	440
$\lvert S_{11}^0\rvert/\nu$	0.007	0.0	0.006	0.0	0.0
$\lvert\hat{h}_2^0\rvert/\nu$	0.0068	0.0057	0.0577	0.1085	0.048
d	0.01	0.01	0.06	0.12	0.06
$\lvert T\rvert$	1.8014	1.7558	1.8828	1.7043	1.8843
$\lvert T\rvert\, d = r_0$	0.018	0.01756	0.1130	0.2045	0.1131

Table 10. Characteristic data determined by the simplified algorithm.

In all cases condition (4.8) is satisfied, and thus, we can conclude that the dimension of the underlying long-time dynamics for tropospheric chemistry model that we discuss in this section can be estimated by 3.

6 Conclusion

In this paper we presented and justified an algorithm that allows us to estimate local dimension of long-time dynamics in multi-scale systems. The special feature that distinguishes this approach from other widely used asymptotic approaches is the following. When using asymptotic reduction algorithms, the dimension of the underlying dynamics is defined in the limit when some small parameters tend to zero (or large parameters tend to infinity). This approach is useful when the corresponding mathematical model is given in the form of a singularly perturbed system (1.2). But in other situations, with given numerical values of coefficients, it is often difficult to decide which parameters are small (large) and which are not, and how the numerical choice of small (large) parameters is related to the procedure of taking the limit and making prediction on the local dimension of slow dynamics. In our approach the local dimension is estimated explicitly for a given problem in terms of given numerical values of coefficients and parameters entering formulation of a problem. The estimate is valid for the vicinity of a particular chosen point of interest, and the size of this vicinity is also determined numerically by the algorithm.
We illustrated the algorithm by applying it to three non-trivial chemical kinetics examples. The results obtained using our algorithm (especially, for the tropospheric chemistry model) are difficult to derive using other methods. These results are not only of theoretical, but also of high practical importance to the researchers working in the area of tropospheric chemistry.
Finally, we would like to mention that, in principle, our local analysis can also be used to derive an algorithm for a dynamic reduction of the dimension of the state space for systems with multiple time-scales. In addition, it can be applied for approximation of invariant manifolds for such systems.

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