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Local state space reduction of multi-scale systems

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Abstract

Modelling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be large. A well-known approach to reduce the dimension of such systems is the quasi-steady state assumption (QSSA): the derivative of fast variables is assumed to be zero. This procedure requires some knowledge of the underlying chemistry, moreover the corresponding differential system must be explicitly given. In this paper we shall describe and justify a procedure for a local reduction of the dimension of state space which does not require chemical insight as well as an explicit knowledge of the system in a singularly perturbed form. The mathematical justification is based on the theory of invariant manifolds.

1 Introduction.

Modelling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be quite large. We assume that the underlying model can be written in the form

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

where z is an n-vector. A well-known approach to reduce the number of differential equations of system (1.1) is the quasi-steady state assumption (QSSA): the derivative of fast variables is assumed to be zero [8, 12, 13]. Consequently, we get a differential-algebraic system which represents under some 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. At the same time we need an explicit knowledge of the corresponding differential system. In case that system (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 solved easily. Under the assumption that the Jacobian $g_y(x,y,t,0)$ is invertible on a solution of $g(x,y,t,0) = 0$, the vector y represents the fast variables near that solution for small ε. If we set $\varepsilon = 0$ then we get from (1.2) 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* to (1.2). If we are able to solve the second equation with respect to y, 1 $y = \varphi(x,t)$, 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* to (1.2) and whose state space has the dimension $m = n - k$. The claim that for sufficiently small positive ε the qualitative behaviour of system (1.2) near the surface $y = \varphi(x,t)$ is determined by the behaviour of system (1.4) can be justified under some conditions by means of the theory of invariant manifolds for singularly perturbed systems [4, 14].

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) with respect to z 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 [6, 7] and by P. Deuflhard and J. Heroth [2] 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 emphasis is devoted to the estimate of the ε-interval for which the manifold exists. Our algorithm to characterize the points in the (x,t)-space where the dimension of the state space of the reaction system (1.1) can be reduced is represented in section 4. In the last section we illustrate our approach by some examples. The first example is a reaction scheme due to P. Duchêne and P. Rouchon [3], the second represents the famous Oregonator. Principally, our local analysis can be also used to derive an algorithm for a dynamic reduction of the dimension of the state space for systems with multiple time-scales, additionally it can be applied to approximate an invariant manifold for such systems.

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 $\alpha \leq t \leq \beta$ satisfying for all t the inequality

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

Then we have for $\alpha \leq t \leq \beta$

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

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 as above where f now satisfies*

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

Then we have for $\alpha \leq t \leq \beta$

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

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

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

From (2.4) we derive

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

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

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

Using (2.4) we get

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

Taking into account the definition of χ we have

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

□

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 find out the fast variables in (1.1). The first step of this procedure is the so-called real Schur decomposition. According to [5] Chapt. 7.4.1 we have:

Proposition 2.1 *To 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. [5] Chapt. 7.6.2). Hence, without loss of generality, we may assume the ordering $Re\ \sigma(R_{ii}) \ge Re\ \sigma(R_{i+1\ i+1})$ for $i = 1, \dots, l-1$.

Now we split the spectrum $\sigma(R)$ of R by means of the splitting parameter $\nu > 0$ into two disjoint sets

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

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 is the block-diagonal structure we are looking for.

3 Existence of an integral manifold of a singularly perturbed system

In this section we prove a theorem on the existence of an integral manifold for a singularly perturbed system with a special structure which plays a fundamental role in our approach. The method to establish this result is basically the same as in [14] but our main goal is to give an estimate of the ε-interval for which the integral manifold exists.

We consider the singularly perturbed system

$$\begin{aligned} \frac{du_1}{dt} &= f(u_1, u_2, t), \\ \varepsilon\,\frac{du_2}{dt} &= Bu_2 + \varepsilon g(u_1, u_2, t) \end{aligned} \tag{3.1}$$

for $0 \le \varepsilon \le \varepsilon^*$ 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 that is, 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 of (3.1) for $0 < \varepsilon \le \varepsilon^*$ with the representation

$$u_2 = \eta^*(u_1, t, \varepsilon) := \varepsilon\varphi(u_1, t) + O(\varepsilon^2)$$

where η^* depends continuously on its variables. We are especially interested to estimate ε^* from below.

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 $D := R^m \times R \times [0, \bar{\varepsilon}]$ continuously into R^k ($\bar{\varepsilon}$ 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 $|A| = \sqrt{\varrho(A^T A)}$ where ϱ denotes the spectral radius.

According to assumption (A_3) there is a constant $c \ge 1$ such that (see [1])

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

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

$$(\mathcal{T}\eta)(u_1^0, t_0, \varepsilon) := \int_{-\infty}^{t_0} X(t_0, \tau, \varepsilon) g(\varphi^\eta(\tau, \varepsilon, u_1^0), \eta(\varphi^\eta(\tau, \varepsilon, u_1^0), \tau, \varepsilon), \tau) d\tau. \tag{3.13}$$

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

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

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

$$|(\mathcal{T}\eta)(u_1^0, t_0, \varepsilon)| \leq \int_{-\infty}^{t_0} c e^{-\gamma(t_0 - \tau)/\varepsilon} c_2 d\tau = \frac{c c_2 \varepsilon}{\gamma}.$$

Now we show that $(\mathcal{T}\eta)(u_1^0, t_0, \varepsilon)$ is lipschitzian in u_1^0. From (3.8) it follows

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

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

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

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

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

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

$$|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^\eta(\tau,\varepsilon,\bar u_1^0)| \le |u_1^0 - \bar u_1^0| + \int_\tau^{t_0} (c_{41}+c_{42}l)|\varphi^\eta(\sigma,\varepsilon,u_1^0) - \varphi^\eta(\sigma,\varepsilon,\bar u_1^0)|d\sigma.$$

According to (2.3) (Lemma 2.2) we have

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

From (3.13), (3.11), (3.4), (3.6), (3.14), (3.16) and (3.18) we obtain

$$\begin{aligned}
&|(\mathcal{T}\eta)(u_1^0,t_0,\varepsilon) - (\mathcal{T}\eta)(\bar u_1^0,t_0,\varepsilon)| \\
\le & \int_{-\infty}^{t_0} c\, e^{-\gamma(t_0-\tau)/\varepsilon} |g(\varphi^\eta(\tau,\varepsilon,u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon),\tau) \\
& -g(\varphi^\eta(\tau,\varepsilon,\bar u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,\bar u_1^0),\tau,\varepsilon),\tau)|d\tau \\
\le & c(c_{51}+c_{52}l)\int_{-\infty}^{t_0} |\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^\eta(\tau,\varepsilon,\bar u_1^0)| e^{-\gamma(t_0-\tau)/\varepsilon} d\tau \\
\le & c(c_{51}+c_{52}l)|u_1^0-\bar u_1^0| \int_{-\infty}^{t_0} e^{-(\gamma-\varepsilon(c_{41}+c_{42}l))(t_0-\tau)/\varepsilon} d\tau = \frac{c\varepsilon(c_{51}+c_{52}l)}{\gamma-\varepsilon(c_{41}+c_{42}l)}|u_1^0-\bar u_1^0|.
\end{aligned}$$

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

$$\begin{aligned}
&|(\mathcal{T}\eta)(u_1^0,t_0,\varepsilon) - (\mathcal{T}\bar\eta)(u_1^0,t_0,\varepsilon)| \\
\le & \int_{-\infty}^{t_0} ce^{-\gamma(t_0-\tau)/\varepsilon} |g(\varphi^\eta(\tau,\varepsilon,u_1^0),\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon),\tau) \\
& -g(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\bar\eta(\varphi^{\bar\eta}(t_0,\varepsilon,u_1^0),\tau,\varepsilon),\tau)|d\tau \\
\le & c\int_{-\infty}^{t_0} e^{-\gamma(t_0-\tau)/\varepsilon}\Big(c_{51}|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)| \\
& +c_{52}(|\eta(\varphi^\eta(\tau,\varepsilon,u_1^0),\tau,\varepsilon) - \eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon)| \\
& +|\eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon) - \bar\eta(\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0),\tau,\varepsilon)|\Big)d\tau \\
\le & c(c_{51}+c_{52}l)\int_{-\infty}^{t_0} e^{-\gamma(t_0-\tau)/\varepsilon}|\varphi^\eta(\tau,\varepsilon,u_1^0) - \varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)|d\tau \\
& +\frac{c\varepsilon c_{52}}{\gamma}||\eta-\bar\eta||.
\end{aligned} \tag{3.19}$$

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

$$\begin{aligned}
&|\varphi^\eta(\tau,\varepsilon,u_1^0)-\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)|\\
\le\ &\int_\tau^{t_0}|f(\varphi^\eta(s,\varepsilon,u_1^0),\eta(1\varphi^\eta(s,\varepsilon,u_1^0),s,\varepsilon),s)-f(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),\bar\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon),s)|ds\\
\le\ &\int_\tau^{t_0}\Big(c_{41}|\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^{\bar\eta}(s,\varepsilon,u_1^0)|+c_{42}(|\eta(\varphi^\eta(s,\varepsilon,u_1^0),s,\varepsilon)-\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon)|\\
&+|\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon)-\bar\eta(\varphi^{\bar\eta}(s,\varepsilon,u_1^0),s,\varepsilon)|\Big)ds\\
\le\ &\int_\tau^{t_0}\Big((c_{41}+c_{42}l)|\varphi^\eta(s,\varepsilon,u_1^0)-\varphi^{\bar\eta}(s,\varepsilon,u_1^0)|\Big)ds+c_{42}||\eta-\bar\eta||(t_0-\tau).
\end{aligned}$$

According to Lemma 2.2 we have

$$|\varphi^\eta(\tau,\varepsilon,u_1^0)-\varphi^{\bar\eta}(\tau,\varepsilon,u_1^0)|\le\frac{c_{42}||\eta-\bar\eta||}{c_{41}+c_{42}l}\Big(\ e^{(c_{41}+lc_{42})(t_0-\tau)}-1\Big). \tag{3.20}$$

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

$$\begin{aligned}
&|(\mathcal{T}\eta)(u_1^0,t_0,\varepsilon)-(\mathcal{T}\bar\eta)(u_1^0,t_0,\varepsilon)|\\
\le\ &\frac{c(c_{51}+lc_{52})}{c_{41}+lc_{42}}\ c_{42}||\eta-\bar\eta||\int_{-\infty}^{t_0}e^{-\gamma(t_0-\tau)/\varepsilon}(e^{(c_{41}+lc_{42})(t_0-\tau)}-1)d\tau+\frac{c\varepsilon c_{52}}{\gamma}||\eta-\bar\eta||\\
=\ &\Big(\frac{\varepsilon^2c(c_{51}+lc_{52})c_{42}}{\gamma(\gamma-\varepsilon(c_{41}+lc_{42}))}+\frac{c\varepsilon c_{52}}{\gamma}\Big)\ ||\eta-\bar\eta||=\frac{c\varepsilon}{\gamma}\Big(\frac{\varepsilon(c_{51}+lc_{52})c_{42}}{\gamma-\varepsilon(c_{41}+c_{42}l)}+c_{52}\Big)||\eta-\bar\eta||.
\end{aligned}$$

□

From Lemma 3.1 and Lemma 3.2 and 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*

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

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 fulfilled 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* $C(d, l)$.

To 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 shall 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

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

Let us introduce the notation

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

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

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

To prove $\varepsilon_2(l) \le \varepsilon_4(l)$ for $l \ge 0$ is equivalent to establish

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

This inequality holds if we have

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

The validity of (3.24) follows from the obvious inequality

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

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

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

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)

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

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

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

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

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

Now we describe our procedure to reduce the dimension of the state space of system (4.1) near (z_0, t_0) by means of Theorem 3.1.

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)).

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 $S^0 = \text{diag}\ (S_{11}^0, S_{22}^0)$ 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 $\varepsilon_\nu := \nu^{-1},\ \gamma = 1$.

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 $e^{B(t-\tau)/\varepsilon}$.

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 $c_2, ..., c_{52}$ 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 as 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 case that 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.

5.1 Example by Duchêne/Rouchon

The following simple reaction scheme has been considered in [3]:

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

where X_1, X_2, X_3 are chemical species, and k_1, k_2, and δk_0 are kinetic constants. The small parameter $\delta > 0$ is used to indicate that the third reaction is slow with respect to 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 (5.1) we shall prove the existence of an invariant manifold for (5.1) and derive an asymptotic approximation of it.

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 it 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

$$
\begin{aligned}
\frac{dy_1}{d\tau} &= -\frac{k_0k_1k_2}{(k_1+k_2)^2}y_1^2 + \frac{k_0(k_1-k_2)}{k_1+k_2}y_1w_2 + k_0w_2^2, \\
\delta\,\frac{dw_2}{d\tau} &= -(k_1+k_2)w_2 - \frac{\delta k_1}{k_1+k_2}\Big\{-\frac{k_0k_1k_2}{(k_1+k_2)^2}y_1^2 + \frac{k_0(k_1-k_2)}{k_1+k_2}y_1w_2 + k_0w_2^2\Big\}
\end{aligned}
\tag{5.4}
$$

possessing 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 fulfilled for sufficiently small δ. Thus, (5.4) has an invariant manifold of $\mathcal{M}_\delta$ the form

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

A straightforward computation yields

$$\varphi_1(y_1) := \frac{k_0k_1^2k_2}{(k_1+k_2)^4}y_1^2,$$

hence we have

$$w_2 = \delta\frac{k_0k_1^2k_2}{(k_1+k_2)^4}y_1^2 + O(\delta^2).$$

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

$$x_2 = \frac{k_1}{k_1+k_2}(x_1+x_2)\Big(1+\delta\frac{k_0k_1k_2}{(k_1+k_2)^3}(x_1+x_2)+O(\delta^2)\Big). \tag{5.5}$$

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. To this end we fix the parameters as

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

such 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 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

Now we test by using our simplified approach whether these points are near an exponentially attracting integral manifold of system (5.1) such that the dimension of the phase space may be reduced.
By means of the coordinate transformation described in section 4 we get from (5.1) for each initial point the following systems in the form (4.5).

Case I_0

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

case II_0

$$\begin{aligned}\frac{du_1}{dt} &= -0.1803 - 0.1383u_1 - 0.0333u_1^2 - 0.0115u_1u_2 + 0.0368u_2^2 \\ \frac{du_2}{dt} &= -6.9053 - 5.0617u_2 + 0.0269u_1^2 + 0.0093u_1u_2 - 0.0297u_2^2,\end{aligned}$$

case III_0

$$\begin{aligned}\frac{du_1}{dt} &= -0.2803 - 0.1532u_1 - 0.0345u_1^2 - 0.0147u_1u_2 + 0.0374u_2^2 \\ \frac{du_2}{dt} &= -6.3552 - 4.8968u_2 + 0.0270u_1^2 + 0.0115u_1u_2 - 0.0293u_2^2\end{aligned}$$

case IV_0

$$\begin{aligned}\frac{du_1}{dt} &= -0.0333u_1^2 - 0.0144u_1u_2 + 0.0375u_2^2 \\ \frac{du_2}{dt} &= -5.0000u_2 + 0.0256u_1^2 + 0.0111u_1u_2 - 0.0288u_2^2.\end{aligned}$$

As neighborhood Σ_d of the origin 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 $\varepsilon_\nu^{-1} = \nu = |\lambda_2|$ such that we have $\gamma = 1$. Obviously it holds $c = 1$, 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
$\lvert S_{11}^0\rvert$	0.3704	0.1383	0.1532	0
$\lvert S_{11}^0\rvert/\nu$	0.0722	0.0273	0.0313	0
$\lvert\hat{h}_2^0\rvert$	14.8091	6.9053	6.3552	0
$\lvert\hat{h}_2^0\rvert/\nu$	2.8870	1.3642	1.2978	0
$\lvert T\rvert$	1.0876	1.1011	1.0765	1.1049
$\lvert T\rvert\, d = r_0$	0.3263	0.3303	0.3229	0.3315

Table 2

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

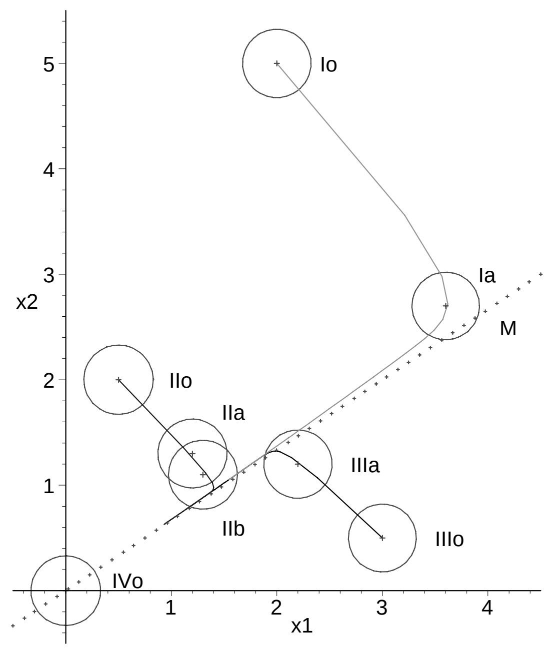

Figure 1

Figure 1 shows the invariant manifold M (dotted line) and the solutions of (5.1) to the start points I_0 - IV_0. It can be seen that corresponding trajectories tends to the curve M which is the zeroth-order approximation of the attracting invariant manifold $\mathcal{M}_\delta$, and that the origin is located on M. The balls centered at the corresponding points have the radius $r_0 = |T|\, d$. We should note that T, and hence also 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 trajectory to 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

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
$\lvert S_{11}^0\rvert$	0.3084	0.1262	0.1182	0.1613
$\lvert S_{11}^0\rvert/\nu$	0.0622	0.0252	0.0237	0.0325
$\lvert\hat{h}_2^0\rvert$	0.6745	1.9989	0.8927	1.2668
$\lvert\hat{h}_2^0\rvert/\nu$	0.1369	0.3995	0.1788	0.2555
$\lvert T\rvert$	1.0711	1.0943	1.0933	1.0846
$\lvert T\rvert\, d = r_0$	0.3213	0.3283	0.3279	0.3254

Table 4

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. 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 [9]

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

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

$$
\begin{aligned}
P^u &= (0,0,0), \\
P^s &= (x_1^s, x_2^s, x_3^s)
\end{aligned}
$$

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 [9]. 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 $\mathcal{M}_\delta$ [10, 11]. 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 $0 < x_2 \le 1$ 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. This curve is represented in Figure 2 as dotted line.

Now we consider the 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

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

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

Analogous systems we get 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	$\|\lambda_2\|$	$\|\lambda_3\|$	$\|\lambda_3\|$	$\|\lambda_3\|$
$\|S_{11}^0\|$	2.5559	240005	8.9775	5.3791
$\|S_{11}^0\|/\nu$	0.6478	$1.64 \cdot 10^{-5}$	$8.9649 \cdot 10^{-4}$	$2.5368 \cdot 10^{-3}$
$\|\hat{h}_2^0\|$	130897	130897	1903.9	0
$\|\hat{h}_2^0\|/\nu$	33176	0.5445	0.1901	0
$\|T\|$	8.4057	8.4057	5.1049	2.8256
$\|T\|\, d = r_0$	0.0083	0.0083	0.0051	0.0028

Table 6

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 algorith says that in a ball with radius 0.003 centered at the equlibrium 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 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

Table 8 contains the corresponding data as well as the results of the simplified algorithm applied to these new points

	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
$\lvert S_{11}^0\rvert$	0.9975	0.1010
$\lvert S_{11}^0\rvert/\nu$	$2.4912 \cdot 10^{-5}$	$2.1959 \cdot 10^{-5}$
$\lvert\hat{h}_2^0\rvert$	5.9959	5.4394
$\lvert\hat{h}_2^0\rvert/\nu$	$1.4975 \cdot 10^{-4}$	$1.1823 \cdot 10^{-4}$
$\lvert T\rvert$	10.1441	2.6543
$\lvert T\rvert\, d = r_0$	0.0101	0.0027

Table 8

Now, in both cases the conditions (4.8) are fulfilled 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. In Fig. 2 these points are represented together with the curve k. The corresponding balls cannot be represented since the radius is too small).

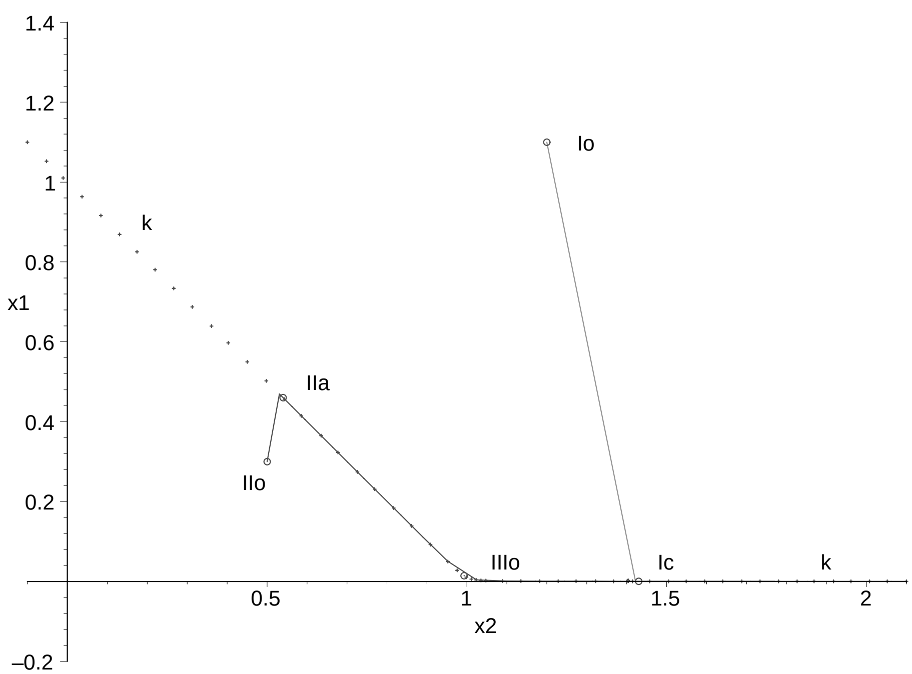

Figure 2

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