A constructive approach to quasi-steady state reductions

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Abstract

We present a method to determine the reduction of a (polynomial or rational) ordinary differential equation that models a chemically reacting system, under the assumption that this system admits quasi-steady state behavior for certain variables or reactions. We interpret quasi-steady state mathematically as a singular perturbation setting to which the classical theorems of Tikhonov and Fenichel apply. Based on a special decomposition of the fast part of the equation, we obtain an explicit formula for a reduced system, defined on the slow manifold (which is a subset of an algebraic variety). Moreover we determine appropriate initial values for the reduced system, which correspond to first integrals of the fast subsystem. These first integrals may not be obtainable in closed form, but locally Taylor expansions are available. We give several examples and applications, and we discuss in detail the separation of a system into fast and slow reactions. It turns out that methods and results from (algorithmic) commutative algebra and algebraic geometry are useful tools for quasi-steady state reduction.

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1 Introduction

Quasi-steady state (QSS) phenomena occur frequently for differential equations that model chemical and biochemical reactions. Their existence, on the one hand, must be taken into account due to stiff behavior for numerical solutions. On the other hand, QSS scenarios are welcome because they permit a (sometimes substantial) reduction of dimension for a given system. By now it is customary to interpret QSS as a singular perturbation phenomenon (Heineken, Tsuchiya and Aris [21], Schauer and Heinrich [34], Segel and Slemrod [35], Kaper and Kaper [25], Goussis [20], and others), and in the present paper we

will adhere to this interpretation. Thus mathematically we work within the framework of Tikhonov's [39] and Fenichel's [14] classical papers. (We will refer to this as *Tikhonov-Fenichel reduction*.) Moreover we will restrict attention to systems with polynomial or rational right-hand side; this is motivated by our focus on chemically reacting systems and mass-action kinetics. This assumption will allow the employment of algebraic techniques.

Tikhonov's theorem (see Verhulst [40], Ch. 8) is directly applicable only if the variables are separated into fast and slow ones. Fenichel's theory [14] overcomes this problem but generally no explicit reduction is given. For systems that model chemical reactions, with additional assumptions, explicit reduction formulas were obtained by Schauer and Heinrich [34], Stiefenhofer [37], Bothe [6], Lee and Othmer [28], among others. Lee and Othmer also discuss the fast initial phase and the determination of appropriate initial values for the reduced system. For general differential equations with rational right-hand side, the principal result in [32] states that whenever the hypotheses of Tikhonov's theorem are satisfied (for suitable coordinates which need not be known explicitly), there exists a reduced system which has again rational right-hand side. However, although the reduction procedure given in [32] is in principle constructive, it is not feasible beyond small dimensions.
In the present paper we start from a QSS scenario, thus a rational system depending on a "small parameter" ε is given which satisfies the hypotheses of Tikhonov's theorem, up to some coordinate transformation. We show that there exists a decomposition of the fast part which generalizes the matrix-vector decomposition obtained from stoichiometry for certain classes of reaction equations (Schauer and Heinrich [34], Bothe [6], Lee and Othmer [28]), but our proof works with (and requires) mathematical arguments only. (The necessary algebraic background is presented in an Appendix, as are some proofs; using these results in applications is quite straightforward.) Once this decomposition (which is obtainable in an algorithmic manner) is known, a reduced system is explicitly computable; in this sense our approach is constructive. We arrive at a reduced system that has rational right-hand side and is defined on an algebraic variety. It may be worth emphasizing that this setting is a natural consequence of mass action kinetics and the Tikhonov-Fenichel reduction procedure; no further assumptions or simplifications are involved. While the determination of the reduced system is thus algorithmically accessible, a discussion of the fast subsystem, hence of the initial phase and the appropriate initial data on the slow manifold, may be more complicated. The fundamental problem is that, although the existence of certain (independent) first integrals for the fast system is known from theory, their explicit determination is generally impossible. (In the special cases discussed by Schauer and Heinrich [34], Bothe [6], Lee and Othmer [28], stoichiometry provides sufficiently many independent linear first integrals.) Generally, resorting to Taylor expansion will yield at least locally useful approximations.

The paper is organized as follows. In Section 2 we briefly review the setup for

singular perturbations, then state a theorem which describes a computationally feasible approach to the reduced equation, which is generally defined on a local submanifold or subvariety of phase space. (The theorem generalizes the main result of [18], which corresponds to the subvariety being an affine subspace. It was announced in [19], but no proof of the crucial part was given there.) We also compare the reduction to existing work in the literature. We proceed to discuss the fast dynamics, in view of determining an appropriate starting value on the slow manifold from given initial data, and then illustrate the method by a number of examples. (More examples are contained in [19].) In Section 3 we turn to the setting of slow and fast reactions (QSS for reactions, or PEA) and discuss the relevance of the classical results by Horn and Jackson, and Feinberg, on Tikhonov-Fenichel reduction. In Section 4 we discuss an example (maltose transport), where reduction leads to a system on a nontrivial algebraic curve. We show that (and how) the behavior of the reduced system can be discussed rather easily in such a setting. An Appendix contains some basic information on algebraic notions, results and algorithms, and also the proof of the main theorem.

2 Reduction

2.1 Preliminaries

Throughout this paper let $U \subset \mathbb{R}^n$ be an open set, $\varepsilon_0 > 0$, and $h\colon U \times [0, \varepsilon_0) \to \mathbb{R}^n$ an analytic function which defines a parameter-dependent system of ordinary differential equations

$$\dot{x} = h^{(0)}(x) + \varepsilon h^{(1)}(x) + \varepsilon^2 \dots , \quad x \in U. \tag{1}$$

The equation may (as reaction equations typically do) depend on further parameters, but we will assume that these are constant, and will suppress them in the notation. In the slow time scale $\tau = \varepsilon t$ we have a singularly perturbed system

$$x' = \frac{1}{\varepsilon} h^{(0)}(x) + h^{(1)}(x) + \varepsilon \dots , \quad x \in U. \tag{2}$$

Our primary interest lies in the behavior as $\varepsilon \to 0$; $h^{(0)}$ will be called the fast part and $h^{(1)}$ the slow part of either system. We will focus on those scenarios for which the classical singular perturbation theorems of Tikhonov [39] and Fenichel [14] hold.

Tikhonov's theorem (specialized to the autonomous analytic case) refers to a system in what we call *Tikhonov standard form*, i.e.,

$$\begin{aligned} y_1' &= f(y_1, y_2) + \varepsilon \dots , & y_1 \in D, \\ \varepsilon y_2' &= g(y_1, y_2) + \varepsilon \dots , & y_2 \in G \end{aligned} \tag{3}$$

in slow time with small parameter $\varepsilon \geq 0$, defined on an open set $D \times G \subset \mathbb{R}^{s+r}$ with $r + s = n$. See the monograph by Verhulst [40]; in particular Theorem 8.1.

Thus, we let

$$\widetilde{Z} := \left\{(y_1,\, y_2)^T \in D \times G;\, g(y_1,\, y_2) = 0\right\}$$

and assume a uniform linear stability condition for the eigenvalues of the Jacobian $D_2 g(y_1,\, y_2)$ (with respect to y_2); viz., the existence of $\mu > 0$ such that

$$\text{Re Sp } D_2 g(y_1,\, y_2) \leq -\mu \quad \text{for every } (y_1,\, y_2) \in \widetilde{Z}. \tag{4}$$

Then Tikhonov's theorem guarantees that there are $T > 0$ and a neighborhood of $\widetilde{Z}$ such that all solutions of (3) starting in this neighborhood converge uniformly on $[t_0,\, T]$ to solutions of the reduced system on $\widetilde{Z}$, given by

$$\dot{y}_1 = f(y_1,\, y_2), \quad g(y_1,\, y_2) = 0 \tag{5}$$

for $\varepsilon \to 0$, for any $t_0 > 0$. We will refer to $\widetilde{Z}$ as the *(asymptotic) slow manifold* of the system.

In general, reaction equations (1) are not in standard form (3). Fenichel [14] deals with this general setting, and the following local characterization of systems which admit a coordinate transformation to Tikhonov standard form essentially goes back to his work. An elementary proof of the next result is given in [32].

Proposition 1. *Let system* (1) *be given, and denote by Z the zero set of $h^{(0)}$. Let $x_0 \in Z$ and assume that there exists a neighborhood $\widetilde{U}$ such that $Z \cap \widetilde{U}$ is an s-dimensional submanifold of $\mathbb{R}^n$. Then there exists an invertible coordinate transformation to standard form* (3) *satisfying condition* (4) *in some neighborhood of x_0, if and only if the following hold.*

(i) The rank of $Dh^{(0)}(x_0)$ is equal to s, and one has a direct sum decomposition

$$\mathbb{R}^n = \text{Ker } Dh^{(0)}(x_0) \oplus \text{Im } Dh^{(0)}(x_0). \tag{6}$$

(ii) The nonzero eigenvalues of $Dh^{(0)}(x_0)$ have real part < 0.

Extending the nomenclature from above, we will refer to $Z \cap \widetilde{U}$ – and briefly to Z – as the (asymptotic) slow manifold of (1).

As pointed out in [32], Proposition 1 guarantees the existence of a transformation to Tikhonov standard form, but generally it is impossible to determine such a transformation explicitly. On the other hand, it was also shown in [32] that a reduced system can be determined explicitly, but some issues of feasibility remained open.

2.2 Reduction of rational systems

We will (have to) use some notions and results from classical commutative algebra and algebraic geometry. For the reader's convenience, a short overview is given in the Appendix, A.1. Our main result provides an algorithmic approach to the computation of reduced equations for general systems (1) with rational

right-hand side, in particular for reaction equations with mass action kinetics. The central argument underlying the reduction theorem relies on a classical result from algebraic geometry; see Lemma 2 in Appendix A.2.

Thus we assume that h is rational, in particular $h^{(0)} \in \mathbb{R}(x)^n$. Hence the zero set $\mathcal{V}(h^{(0)})$ forms a Zariski-open and dense subset of an algebraic variety. The following result describes Tikhonov-Fenichel reduction in such a scenario.

Theorem 1. *Consider system* (1) *with rational right-hand side h, and let $a \in \mathbb{R}^n$ be a simple point of $\mathcal{V}(h^{(0)})$, with $r = \operatorname{rank}\, Dh^{(0)}(a)$. (Thus locally the dimension of $\mathcal{V}(h^{(0)})$ equals $s = n - r$.) Assume moreover that there is a direct sum decomposition*

$$\mathbb{R}^n = \operatorname{Ker}\, Dh^{(0)}(a) \oplus \operatorname{Im}\, Dh^{(0)}(a).$$

Then the following hold.

(a) There exist a Zariski-open neighborhood U_a of a in $\mathbb{R}^n$ and a product decomposition with matrices $\mu(x) \in \mathbb{R}(x)^{r\times 1}$, $P(x) \in \mathbb{R}(x)^{n\times r}$, such that

$$h^{(0)}(x) = P(x)\mu(x), \quad x \in U_a \tag{7}$$

with $\operatorname{rank}\, P(a) = r$, $\operatorname{rank}\, D\mu(a) = r$ *and*

$$\mathcal{V}(h^{(0)}) \cap U_a = \mathcal{V}(\mu) \cap U_a$$

is a $(n-r)$–dimensional submanifold. The entries of μ may be taken as any r entries of $h^{(0)}$ that are functionally independent at a.

(b) The following system is defined on a Zariski-open neighborhood of a in $\mathbb{R}^n$, and admits a Zariski-open neighborhood $\mathcal{U}_a \subset \mathcal{V}(h^0)$ as an invariant set:

$$x' = \left[I_n - P(x)A(x)^{-1}D\mu(x)\right] h^{(1)}(x), \tag{8}$$

with

$$A(x) := D\mu(x)P(x) \in \mathbb{R}(x)^{r\times r}$$

invertible for all $x \in \mathcal{U}_a$.

(c) If all the nonzero eigenvalues of $Dh^{(0)}(a)$ have negative real part then system (8)*, restricted to the slow manifold $\mathcal{U}_a$, corresponds to the reduced system* (5) *from Tikhonov's theorem.*

The proof of this Theorem will be given in Appendix A.2.

Remark 1. (a) We will call

$$Q(x) := I_n - P(x)A(x)^{-1}D\mu(x) \tag{9}$$

the *projection operator* of the reduction. Although this may seem apparent from (8), it is not necessary to invert the matrix $A(x)$; in practice one only needs to solve one linear system of equations involving this matrix. The size $(r \times r)$ of A determines the size of the reduction (to a system of dimension $n - r$).

(b) The projection operator Q projects $h^{(1)}(x)$ to its kernel component in the kernel-image decomposition with respect to $Dh^{(0)}(x)$. This corresponds to the reduced system in the sense of Tikhonov and Fenichel, as shown in [32], Lemma 2.4 and Proposition 2.5. One may also view this projection as a special (degenerate) instance of the CSP reduction by Lam and Goussis [27], where a decomposition corresponding to "large" and "small' eigenvalues is carried out iteratively. In the limiting case when the small eigenvalues are equal to zero (and one has a direct kernel-image decomposition), the iteration terminates after one step.

(c) A detailed proof of part (b) is given in [19]. The specific form of the reduced system for particular classes of equations – using special properties of reaction equations and with different proofs – was also given earlier by Boulier et al. [5], and (in a special case) by Bothe [6], Theorem 2; see also Lee and Othmer [28]. The classical paper by Fenichel [14], as well as Stiefenhofer's paper [37], contain explicit reduction formulas for sufficiently smooth vector fields under the assumption that a parameterization of the slow manifold is explicitly known. The crucial point of our approach, however, is the general existence of the decomposition in part (a); we prove this by a purely mathematical argument.

(d) There is a constructive method to obtain the multiplicative decomposition in part (a) of the Theorem, and thus the reduction procedure as a whole is algorithmically accessible. The argument is sketched in Appendix A.3. We note that in many applications one will find a decomposition by inspection.

Remark 2. Theorem 1 also applies to the analytic (and to the sufficiently smooth) case. In these settings the decomposition in part (a) is a consequence of the implicit function theorem; the proof of part (b) rests only on the existence of such a decomposition. But note that generally this is not a constructive approach.

Remark 3. (a) The right-hand side of (8) is well-defined whenever the direct sum decomposition of $\mathbb{R}^n$ with respect to $Dh^{(0)}(a)$ exists; we will sometimes refer to this as a *formal reduction*. The results of Fenichel [14] show that there actually exists a slow manifold (not attractive in general) provided that all nonzero eigenvalues of $Dh^{(0)}(a)$ have nonzero real part (the normally hyperbolic case). The following observation, which goes back to a statement of Tikhonov's theorem with weaker hypotheses (see e.g. Verhulst [40], Thm. 8.1, hypothesis b) is also worth noting: If every point a in a neighborhood of a_0 in $\mathcal{V}(h^{(0)})$ is asymptotically stable for the equation $\dot{x} = h^{(0)}(x)$, with attraction locally uniform in a, then one has a convergence result analogous to part (c) of the Theorem.

(b) The condition, in Theorem 1, on a being a simple point of the variety $\mathcal{V}(h^{(0)})$ is also necessary for the existence of a reduction in the sense of Tikhonov and Fenichel, since it is necessary for the local submanifold property. We

do not address the (interesting) question of behavior near singular points in this paper.

Remark 4. It may be appropriate to take a closer look at the linear algebra underlying part (b) of Theorem 1. Thus let $r < n$ and $R \in \mathbb{R}^{n\times n}$ of rank r, $S \in \mathbb{R}^{n\times r}$ and $T \in \mathbb{R}^{r\times n}$ such that

$$R = ST.$$

Then $\operatorname{rank} T = r$ and $\operatorname{Ker} R = \operatorname{Ker} T$, $\operatorname{Im} R = \operatorname{Im} S$, and the following are equivalent.

(i) $\mathbb{R}^n = \operatorname{Ker} R \oplus \operatorname{Im} R$;
(ii) $\mathbb{R}^n = \operatorname{Ker} T \oplus \operatorname{Im} S$;
(iii) $\operatorname{Ker} T \cap \operatorname{Im} S = \{0\}$;
(iv) TS is invertible.

These statements and their proofs are standard. For instance, the first assertion is a consequence of $\operatorname{rank} ST \leq \min\{\operatorname{rank} S, \operatorname{rank} T\}$, and the second follows from $\operatorname{Ker} R \subseteq \operatorname{Ker} T$ and equal dimension. This underlies Theorem 1(b), with $R = Dh^{(0)}(x)$, $S = P(x)$, $T = D\mu(x)$ for $x \in \mathcal{V}(h^{(0)})$. We will get back to such arguments in Section 3.

2.3 Fast dynamics

We turn to the initial phase for system (1), given that the conditions of Proposition 1 are satisfied. Our principal interest lies in determining appropriate initial data for the reduced system (8) from the initial data of (1). Tikhonov's theorem is – again – crucial for this, thus we first review the setting in Tikhonov standard form.
In fast time, system (3) becomes

$$\begin{aligned} \dot{y}_1 &= \varepsilon f(y_1, y_2) + \varepsilon^2 \ldots, & y_1 \in D \subset \mathbb{R}^s \\ \dot{y}_2 &= g(y_1, y_2) + \varepsilon \ldots, & y_2 \in G \subset \mathbb{R}^r, \end{aligned} \tag{10}$$

which in the limiting case $\varepsilon = 0$ degenerates to the system

$$\begin{aligned} \dot{y}_1 &= 0 \\ \dot{y}_2 &= g(y_1, y_2), \end{aligned}$$

which has two characteristic features: Every entry of y_1 is a first integral, and every solution of this equation, starting at (z_1, z_2) in a sufficiently small neighborhood of the slow manifold $\widetilde{Z}$, converges for $t \to \infty$ to a single point on $\widetilde{Z}$, which is defined by $g(z_1, y_2^*) = 0$. In other words, the limit point is the intersection of $\widetilde{Z}$ and level sets of first integrals. By coordinate change and Proposition 1 we obtain:

Proposition 2. *Let $x_0 \in \mathcal{V}(h^{(0)})$ and suppose that there is some neighborhood $\widetilde{U}$ of x_0 such that $\mathcal{V}(h^{(0)}) \cap \widetilde{U}$ is an s-dimensional submanifold of $\mathbb{R}^n$. Moreover assume that conditions (i) and (ii) in Proposition 1 are satisfied. Then the following hold for $\varepsilon = 0$.*

(a) System (1) *admits s independent first integrals $\phi_1, \ldots, \phi_s$ in a neighborhood U^* of x_0. Moreover, in U^* the intersection of every level set $\phi_j(x) = c_j =$* const.*, $1 \le j \le s$, with $\mathcal{V}(h^{(0)})$ consists of a single point.*

(b) For any $w \in U^*$ which also lies in the domain of attraction, the solution of (1) *with initial value w converges to the intersection point of $\mathcal{V}(h^{(0)})$ and the level set $\phi_j(x) = \phi_j(w)$, $1 \le j \le s$, as $t \to \infty$.*

This intersection point is the appropriate initial value for the reduced system on the slow manifold, which approximates the behavior of (1) for small $\varepsilon > 0$. For a proof see Fenichel [14], Theorem 9.1, and also the arguments in Verhulst [40], Section 8.3, about matching of expansions. Moreover, cf. Lee and Othmer [28], p. 404f. and p. 407f.; and Stiefenhofer [37], p. 596 and p. 599 for reaction systems.

Remark 5. In the context of reaction equations the determination of appropriate initial data on the slow manifold has been discussed by Heinrich and Schauer [34], Stiefenhofer [37], and Lee and Othmer [28] (in particular p. 408). They consider a slow–fast reaction scenario and make specific use of linear first integrals given by stoichiometric properties of the fast subsystem. Stiefenhofer [37], p. 607 discusses an application to a maltose transport model. See Section 3 for more details.

Remark 6. Generally one cannot determine first integrals of the fast subsystem explicitly; see the discussion about transformations to Tikhonov standard form in [32]. But one can determine Taylor approximations of such first integrals near the slow manifold Z. Thus let $x_0 \in Z$ be a simple point. Then $h^{(0)}$ admits a Taylor expansion

$$h^{(0)}(x) = h_1^{(0)}(x - x_0) + h_2^{(0)}(x - x_0) + \ldots$$

with homogeneous terms $h_j^{(0)}(x - x_0)$ of degree j. An analytic first integral ψ of $h^{(0)}$ has a representation

$$\psi(x) = \psi_1(x - x_0) + \psi_2(x - x_0) + \ldots$$

with homogeneous ψ_i of degree i. Since ψ is a first integral, the Lie derivative with respect to $h^{(0)}$ vanishes, thus

$$\left(L_{h^{(0)}}\psi\right)(x) = D\psi(x)h^{(0)}(x) = 0, \quad \text{for all } x.$$

Evaluating this condition degree by degree, one obtains necessary and sufficient conditions

$$\begin{array}{ll} \text{Degree } 1: & D\psi_1(y)h_1^{(0)}(y) = 0 \\ \text{Degree } 2: & D\psi_2(y)h_1^{(0)}(y) + D\psi_1(y)h_2^{(0)}(y) = 0 \\ \text{Degree } 3: & D\psi_3(y)h_1^{(0)}(y) + D\psi_2(y)h_2^{(0)}(y) + D\psi_1(y)h_3^{(0)}(y) = 0 \\ & \vdots \end{array} \tag{11}$$

For given $h_j^{(0)}$ this allows a successive determination of the ψ_i; the existence of s independent solutions (i.e., s linearly independent initial terms of degree one) is guaranteed by [32], for instance.
The approximations thus obtained are relevant at least for initial values close to the slow manifold. The computations can be handled by any standard algorithmic algebra software.

2.4 Examples

Several applications of Theorem 1, including reversible Michaelis-Menten and generalizations, have been discussed in [18] (where a special case of Theorem 1 was considered), and in [19]. We present more examples here, for some including a discussion of the initial phase. Our main purpose is to illustrate the reduction procedure.

Example 1. Consider the reaction scheme

$$\begin{array}{rcl} X+Y & \underset{\varepsilon\kappa_{-1}}{\overset{k_1}{\rightleftharpoons}} & Z, \\ X & \overset{k_2}{\longrightarrow} & \emptyset, \\ Z & \overset{\varepsilon\kappa_3}{\longrightarrow} & \emptyset, \end{array}$$

imposing a QSS assumption on both reactions starting from Z, thus ε is a small parameter. The reaction equations are given by

$$\frac{d}{dt}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -k_1xy - k_2x \\ -k_1xy \\ k_1xy \end{pmatrix} + \varepsilon \begin{pmatrix} \kappa_{-1}z \\ \kappa_{-1}z \\ -(\kappa_{-1}+\kappa_3)z \end{pmatrix}.$$

We decompose the fast term

$$h^{(0)} = P(x,y,z)\cdot\mu(x,y,z) := \begin{pmatrix} -k_1y - k_2 \\ -k_1y \\ k_1y \end{pmatrix}\cdot x.$$

Since $(D\mu P)(x,y,z) = -k_1y - k_2 < 0$ for all $y \geq 0$, the convergence conditions in Theorem 1 are satisfied on the nonnegative part of the slow manifold $W := \mathcal{V}(h^{(0)}) = \{(0,y,z);\, y,z \in \mathbb{R}\}$. As stated in Theorem 1, the reduced system is given by applying the projection

$$Q = I_3 - P(D\mu P)^{-1}D\mu = \begin{pmatrix} 0 & 0 & 0 \\ -\frac{k_1y}{k_1y+k_2} & 1 & 0 \\ \frac{k_1y}{k_1y+k_2} & 0 & 1 \end{pmatrix}$$

to the slow term. Thus we get the reduced dynamics

$$\begin{array}{rcl} \dot{y} & = & \frac{k_{-1}k_2}{k_1y+k_2}z \\ \dot{z} & = & -\left(\frac{k_{-1}k_2}{k_1y+k_2} + k_3\right)z \end{array} \tag{12}$$

on the slow manifold W; as a matter of notational convenience we set $k_{-1} = \varepsilon\kappa_{-1}$ and $k_3 = \varepsilon\kappa_3$.
During the transient phase the initial value $(x_0, y_0, z_0)^T \in \mathbb{R}^3$ in the domain of attraction of $\mathcal{V}(h^{(0)})$ is attracted by a point $(0, y^*, z^*)^T \in \mathcal{V}(\mu)$. Asymptotically the fast dynamics is given by $h^{(0)}$ which has two independent first integrals, viz.

$$\psi_1((x,y,z)^T) = k_1(x-y) - k_2 \ln y \quad \text{and} \quad \psi_2((x,y,z)^T) = y + z.$$

The second of these is due to stoichiometry, while the first can be obtained from the separable orbit equation

$$\frac{dx}{dy}(= \frac{\dot{x}}{\dot{y}}) = 1 + \frac{k_2}{k_1} \cdot \frac{1}{y}.$$

Accordingly, y^* and z^* are uniquely determined by

$$\begin{array}{rcl} y^* + z^* & = & y_0 + z_0, \\ k_1 y^* + k_2 \ln y^* & = & k_1(y_0 - x_0) + k_2 \ln y_0. \end{array} \tag{13}$$

(As for uniqueness note that $y \mapsto k_1 y + k_2 \ln y$ is stricly increasing.) To summarize, system (12) gives the reduced dynamics, with initial data determined by (13).

Example 2. Next we discuss the Brusselator model (Prigogine and Lefever [33]) with a QSS assumption for one of the reactions. Consider the reaction scheme

$$\begin{array}{rcl} A & \stackrel{k}{\rightharpoonup} & X, \\ 2X + Y & \stackrel{\ell}{\rightharpoonup} & 3X, \\ B + X & \stackrel{m}{\rightharpoonup} & Y + D, \\ X & \stackrel{n}{\rightharpoonup} & E, \end{array}$$

with rate constants $k, \ell, m, n > 0$. We impose a QSS assumption on the first reaction, thus k is our small parameter. The four-dimensional system of reaction equations is given by

$$\frac{d}{dt}\begin{pmatrix} a \\ x \\ y \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ -\ell x^2 y + \ell x^3 - mbx - nx \\ -\ell x^2 y + mbx \\ -mbx \end{pmatrix} + k \begin{pmatrix} -a \\ a \\ 0 \\ 0 \end{pmatrix},$$

$(a, x, y, b)^T \in \mathbb{R}^4$. (Incidentally, this may also be interpreted as the case of a "slow variable" a.) The fast term $h^{(0)}$ vanishes on the submanifold W given by $x = 0$. Since the Jacobian of the fast term

$$Dh^{(0)}(a, 0, y, b) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -mb - n & 0 & 0 \\ 0 & mb & 0 & 0 \\ 0 & -mb & 0 & 0 \end{pmatrix}$$

has rank one when $x = 0$ and the nontrivial eigenvalue is negative, there exists a Tikhonov-Fenichel reduction to the attractive slow manifold W. Defining

$$P(a,x,y,b) = \begin{pmatrix} 0 \\ -\ell xy + \ell x^2 - mb - n \\ -\ell xy + mb \\ -mb \end{pmatrix}, \quad \mu(a,x,y,b) = x,$$

Theorem 1 yields the reduced 3-dimensional system

$$\begin{aligned} \dot{a} &= -a \\ \dot{y} &= mba/(mb+n) \\ \dot{b} &= -mba/(mb+n) \end{aligned}$$

on W, which is elementary.
We turn to first integrals of

$$h^{(0)} = h_1^{(0)} + h_2^{(0)} + \cdots = \begin{pmatrix} 0 \\ -nx \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ -mbx \\ mbx \\ -mbx \end{pmatrix} + \cdots$$

in order to find appropriate initial values on the slow manifold. According to Proposition 2, three independent first integrals exist near any point of W. One of these is given by the first coordinate $(a,x,y,b) \mapsto a$, but the explicit determination of three independent first integrals of $h^{(0)}$ seems impossible here. Hence we use Remark 6 and determine an approximation up to degree two. Obviously, $(a,x,y,b) \mapsto y$ and $(a,x,y,b) \mapsto b$ are independent first integrals of $h_1^{(0)}$, and Proposition 2 guarantees that there exist first integrals $\phi = y + \text{t.h.o.}$, $\psi = b + \text{t.h.o.}$ for $h^{(0)}$.
Up to degree 2 we make the ansatz

$$\phi(a,x,y,b) = y + \alpha_1 x^2 + \beta_1 xa + \gamma_1 xy + \delta_1 xb + \cdots = \phi_1 + \phi_2 + \text{t.h.o.}$$

with undetermined coefficients of the quadratic terms, and evaluate the condition

$$D\phi_1\, h_2^{(0)} + D\phi_2\, h_1^{(0)} = 0$$

for the homogeneous quadratic part. (In principle there are 10 monomials to be considered in the quadratic part, but any product of two terms a, y and b will provide no information, since a, y and b are initial terms of first integrals, and products of first integrals are first integrals). We get

$$mbx = -2\alpha_1 x^2 - n\beta_1 xa - n\gamma_1 xy - n\delta_1 xb$$

and therefore $\delta_1 = -\frac{m}{n}$, $\quad \alpha_1 = \beta_1 = \gamma_1 = 0$, comparing coefficients. We have

$$\phi(a,x,y,b) = y - \frac{m}{n} bx + \cdots,$$

and by a similar computation

$$\psi(a, x, y, b) = b - \frac{m}{n} bx + \cdots$$

Thus the fast dynamics project an initial point $(a_0, x_0, y_0, b_0)^T$ near W to $(a^*, 0, y^*, b^*)^T \in W$, with

$$a^* = a_0,\ y^* = y_0 - \frac{m}{n} b_0 x_0,\ b^* = b_0 - \frac{m}{n} b_0 x_0,$$

with approximation up to degree 2.

Example 3 (Field-Noyes model)**.** We discuss a Field-Noyes model [15], following the presentation in Murray [31], Ch. 8. The reaction scheme is given by

$$\begin{array}{lll} A + Y \xrightarrow{k_1} X + P, & & X + Y \xrightarrow{k_2} 2P, \\ A + X \xrightarrow{k_3} 2X + 2Z, & 2X \xrightarrow{k_4} A + P, & Z \xrightarrow{k_5} fY \end{array}$$

for some $f \geq 0$. (This scheme is to be understood as compounding a larger set of elementary reactions.) By mass-action kinetics one obtains a four-dimensional differential equation

$$\begin{array}{rcl} \dot{a} &=& -k_1 ay - k_3 ax + k_4 x^2 \\ \dot{x} &=& k_1 ay - k_2 xy + k_3 ax - k_4 x^2 \\ \dot{y} &=& -k_1 ay - k_2 xy + f k_5 z \\ \dot{z} &=& 2k_3 ax - k_5 z \end{array} \tag{14}$$

We will not invoke the additional assumption in Murray [31], p. 260 that a is (nearly) constant (which is used in [31] to reduce the system to three dimensions). Rather we look at one possible interpretation of this assumption: We interpret the requirement of constant a to mean that the function a is a first integral of (14), thus $k_1 = k_3 = k_4 = 0$. We relax these conditions to

$$k_1 = \varepsilon\kappa_1,\ k_3 = \varepsilon\kappa_3,\ k_4 = \varepsilon\kappa_4$$

to obtain "almost-constancy" of a; this yields a slow-fast separation with fast part

$$h^{(0)} = \begin{pmatrix} 0 \\ -k_2 xy \\ -k_2 xy + f k_5 z \\ -k_5 z \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ -k_2 x & 0 \\ -k_2 x & f k_5 \\ 0 & -k_5 \end{pmatrix} \cdot \begin{pmatrix} y \\ z \end{pmatrix}$$

and slow manifold W defined by $y = z = 0$. A Tikhonov-Fenichel reduction to W exists, with

$$A = \begin{pmatrix} -k_2 x & f k_5 \\ 0 & -k_5 \end{pmatrix}, \quad A^{-1} = \rho^{-1} \begin{pmatrix} -k_5 & -f k_5 \\ 0 & -k_2 x \end{pmatrix}; \quad \rho = k_2 k_5 x$$

and projection matrix

$$Q = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & -f \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The reduced system on W is thus given by

$$\begin{aligned} \dot{a} &= -k_3 a x + k_4 x^2 \\ \dot{x} &= (1-2f) k_3 a x - k_4 x^2 \end{aligned}$$

This system exhibits rather simple behavior; for instance $\psi = a + x$ is obviously a Lyapunov function. (One should be aware that at $x = 0$ the reduction is no longer guaranteed, since the rank of P collapses to one. There is also a two-dimensional slow manifold contained in the plane $x = z = 0$, with equally simple dynamics. We refrain from discussing the interplay of these two slow manifold components, such as possible switching of an asymptotic solution from one to the other.)

Example 4. We also provide some systems for which there is no direct sum decomposition as required in Proposition 1, and the reduction procedure is not applicable.

- The first one is rather simple (if a bit contrived), with reaction scheme

  $$X \overset{\varepsilon\kappa_1}{\rightharpoonup} mY, \quad Y \overset{\varepsilon\kappa_2}{\rightharpoonup} \emptyset,$$

  thus X degrades slowly, and every molecule of X degrades to large number m of Y-molecules, which in turn degrade slowly. The specific condition we impose is $m\varepsilon = 1$. Hence the differential equation reads

  $$\begin{aligned} \dot{x} &= -\varepsilon\kappa_1 x \\ \dot{y} &= x - \varepsilon\kappa_2 y, \end{aligned}$$

  with fast part

  $$h^{(0)} = \begin{pmatrix} 0 \\ x \end{pmatrix}, \quad Dh^{(0)} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

  and there is no kernel-image decomposition for this nilpotent matrix (Tikhonov is not applicable in any coordinate system). Likewise, there is no sensible reduction to a "slow manifold" (which would have to be defined by $x = 0$) here. As the explicit solution of this linear system shows, generally solutions do not approach the set $x = 0$ quickly, and the dynamics for y is not adequately described by the "reduced equation" $\dot{y} = -\varepsilon\kappa_2 y$.

- Consider a simple autocatalytic reaction scheme

  $$X + Y \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2X$$

with associated differential equation

$$\begin{aligned} \dot{x} &= k_+ xy - k_- x^2 \\ \dot{y} &= -k_+ xy + k_- x^2. \end{aligned}$$

Assuming that $(-k_- x^2,\, k_- x^2)^T$ is the fast part, we have the one-dimensional slow manifold W defined by $x = 0$. Since the Jacobian vanishes on W, there is no direct sum decomposition with appropriate dimensions.

- The following reaction scheme for a pyrolytic process can be found in the literature; see e.g. Aiken [1], p. 44.

$$\begin{aligned} &X_1 \overset{k_1}{\longrightarrow} X_2 + X_3, \quad X_2 + X_3 \overset{k_2}{\longrightarrow} X_5, \\ &X_1 + X_3 \overset{k_3}{\longrightarrow} X_4, \quad X_4 \overset{k_4}{\longrightarrow} X_3 + X_6. \end{aligned}$$

Through mass action kinetics, first integrals $x_1 + x_3 + 2x_4 + x_5 + x_6$ and $x_2 - x_3 - x_4$, and initial conditions $x_1(0) = c$, $x_j(0) = 0$ for $j > 1$ one arrives at the differential equation

$$\begin{aligned} \dot{x}_3 &= (k_1 - k_3 x_3)\,(c - x_3 - 2x_4 - x_5 - x_6) - k_2 x_3 (x_3 + x_4) + k_4 x_4 \\ \dot{x}_4 &= k_3 x_3\,(c - x_3 - 2x_4 - x_5 - x_6) - k_4 x_4 \\ \dot{x}_5 &= k_2 x_3 (x_3 + x_4) \\ \dot{x}_6 &= k_4 x_4. \end{aligned}$$

Assuming that $k_1 = \varepsilon \kappa_1$ represents the slow part of the reaction, we obtain a two-dimensional slow manifold

$$W = \left\{(0,\, 0,\, x_5,\, x_6)^T\right\}$$

and

$$Dh^{(0)}(0,\, 0,\, x_5,\, x_6) = \begin{pmatrix} -k_3(c - x_5 - x_6) & k_4 & 0 & 0 \\ k_3(c - x_5 - x_6) & -k_4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & k_4 & 0 & 0 \end{pmatrix}$$

Here the algebraic and the geometric multiplicity of the eigenvalue 0 are different; the reduction theorem is not applicable.

3 Slow and fast reactions

3.1 Review of reaction equations

We first briefly sketch the standard procedure to assign to a chemical reaction network (in a spatially homogeneous setting, with constant thermodynamical parameters) a system of ordinary differential equations. The main purpose is to fix notation and recall some pertinent results. More detailed presentations can be found e.g. in Feinberg [13], Sections 2-3, Lee and Othmer [28], Section 2, or Schauer and Heinrich [34], Section 2. We use the terminology from Feinberg

[13].
Suppose that one has *chemical species* $X_1, \ldots, X_n$, with respective concentrations (in suitable units) denoted by $x_1, \ldots, x_n$. A *reaction* is denoted by

$$d_1 X_1 + \cdots + d_n X_n \rightharpoonup e_1 X_1 + \cdots + e_n X_n$$

with nonnegative integers d_j, e_j, and $d_i \neq e_i$ for at least one i. (More generally, one may consider nonnegative real numbers d_j, e_j, and discuss generalized mass-action kinetics.) The formal linear combinations on both sides are called *complexes*; formally, a *reaction* is an ordered pair of complexes. Thus a reaction network may be seen as a directed graph, with complexes as nodes and reactions as edges. The connected components of the underlying undirected graph are called *linkage classes*. A network is called *weakly reversible* if for every directed edge connecting two complexes there is a sequence of directed edges connecting these complexes in reverse order.
The ordinary differential equation assigned to the above reaction (with rate constant $k > 0$) is

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = k x_1^{d_1} \cdots x_n^{d_n} \begin{pmatrix} e_1 - d_1 \\ \vdots \\ e_n - d_n \end{pmatrix}.$$

The vector on the right-hand side is also called a stoichiometric vector. (The stoichiometric vectors span the *stoichiometric subspace* of the network.) To obtain the differential equation for a network of reactions one adds up the individual reaction terms. One may rewrite this concisely as

$$\dot{x} = f(x) := S \cdot \theta(x), \tag{15}$$

with the columns of the *stoichiometric matrix* S being the stoichiometric vectors, and θ a vector-valued function with monomial entries. (There are various notions of stoichiometric matrix, but this is of no consequence for our purpose.)
The *deficiency* of a network is defined as the number of complexes, minus the number of linkage classes, minus the dimension of the stoichiometric subspace; this is always a nonnegative integer. Similarly one defines the deficiency of a single linkage class.
Whenever $\beta : x \mapsto \sum \beta_j x_j$ is a linear form with $(\beta_1, \ldots, \beta_n) \cdot S = 0$ then β is a first integral of (15). We speak of a linear first integral *induced by stoichiometry*.
A *stoichiometric compatibility class* (SCC) is by definition a coset of the stoichiometric subspace which contains an element of $\mathbb{R}^n_+$; it is called positive whenever it contains an element of the interior ${\mathbb{R}^*_+}^n$. Thus stoichiometric compatibility classes may also be seen as common level sets of linear first integrals from stoichiometry.
Addressing the differential equation, one first will simplify the matrix in (15), since the columns of S will generally be linearly dependent (for instance whenever the network contains both a reaction and its reverse). Lee and Othmer [28], Section 3, provide an algorithm for such a simplification. For our purpose the following will suffice.

Lemma 1. *Let* (15) *be given, and* $\operatorname{rank} S = q > 0$.

(a) There exist a matrix $\widehat{P} \in \mathbb{R}^{n\times q}$ *and a polynomial* $\widehat{\mu} \in \mathbb{R}[x]^q$ *such that* $\operatorname{rank} \widehat{P} = q$ *and*

$$f(x) = S \cdot \theta(x) = \widehat{P} \cdot \widehat{\mu}(x).$$

(b) If $W \subseteq \mathcal{V}(f)$ *is a local submanifold of dimension* $n - r \geq n - q$ *then there exists a further decomposition*

$$\widehat{\mu}(x) = P^*(x)\mu(x), \quad f(x) = \widehat{P}P^*(x)\mu(x)$$

with $P^* \in \mathbb{R}(x)^{q\times r}$ *of rank* r, $\mu \in \mathbb{R}[x]^r$, *and* $W = \mathcal{V}(\mu)$ *locally. In the special case* $r = q$ *one may take* $P^* = I_q$.

(c) Assume that $x_0 \in \mathbb{R}^n_+$ *is a stationary point which is isolated in its SCC, and that* $D\widehat{\mu}(x_0)\widehat{P}(x_0)$ *is invertible. Then there is a neighborhood* U *of* x_0 *such that* $W := \mathcal{V}(f) \cap U$ *is a local submanifold of dimension* $n-q$, *and moreover* $\mathbb{R}^n = \operatorname{Ker} Df(x) \oplus \operatorname{Im} Df(x)$ *for all* $x \in W$.

Proof. For part (a), elementary column operations transform S to $(\widehat{P} \,|\, 0)$ with $\widehat{P} \in \mathbb{R}^{n\times q}$ of full rank; in other words there is an invertible $n \times n$ matrix Λ such that

$$S = (\widehat{P} \,|\, 0)\Lambda.$$

Defining $\widehat{\mu}(x)$ as the first q entries of $\Lambda \cdot \theta(x)$, the assertion follows. The proof of part (b) is based on Lemma 2 and similar to that of Theorem 1. For part (c) we use Remark 4 to verify the direct sum decomposition. By the implicit function theorem, the zero set of $\widehat{\mu}$ is locally a submanifold of dimension $n - q$. Since (again by Remark 4) the tangent space of W at x_0 and the subspace spanned by the columns of $\widehat{P}$ have trivial intersection, W coincides locally with the zero set of f. □

Examples 1 and 2 above show that one generally cannot expect a decomposition in the sense of Theorem 1 with constant matrix P; in both cases there are too few linear first integrals. (Note that determining linear first integrals is just a matter of solving a system of linear equations for the coefficients, hence all these can be found explicitly.) Thus the mathematical approach to the decomposition in Theorem 1 goes beyond arguments from stoichiometry. The following example illustrates that there may be an appropriate decomposition with a constant matrix, but the matrix is not obtained from stoichiometry only. (Lee and Othmer [28], Section 3, Step 3, discuss this case generally; there must be linear first integrals which are not induced by stoichiometry.)

Example 5. We consider a model of suicide kinetics, discussed in Burke et al. [8] and Tatsunami et al. [38] (and also in [17]), with reaction scheme

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} X \xrightarrow{k_2} Y \xrightarrow{k_3} E + P, \quad Y \xrightarrow{k_4} E_i$$

for substrate S, enzymes E, E_i, intermediates X, Y and product P. In addition to a Michaelis-Menten scheme with two intermediates, there is also irreversible degradation of Y to inactivated enzyme E_i. Since a molecule of S is irreversibly bound in E_i, one calls S a suicide substrate.
Let $z = (e, s, x, y, p, e_i)^T \in \mathbb{R}^6_+$ denote the vector of concentrations, $\dot{z} = f(z)$ the equations of the suicide kinetics. A stoichiometric decomposition $f(z) = \widehat{P} \cdot \widehat{\mu}(z)$ reads

$$f(z) = \begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} k_1 es + k_{-1} x \\ k_2 x \\ k_3 y \\ k_4 y \end{pmatrix}.$$

Note that the entries of $\widehat{\mu}$ are dependent; the zero set is a union of two three-dimensional subspaces given by $e = x = y = 0$ resp. $s = x = y = 0$. A further decomposition according to Lemma 1 (b) is easy to find:

$$\widehat{\mu} = P^* \cdot \mu := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k_3 \\ 0 & 0 & k_4 \end{pmatrix} \begin{pmatrix} k_1 es + k_{-1} x \\ k_2 x \\ y \end{pmatrix}$$

To summarize, we obtain a decomposition with matrix

$$P := \begin{pmatrix} -1 & 0 & 1 \\ -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -(k_3 + k_4) \\ 0 & 0 & k_3 \\ 0 & 0 & k_4 \end{pmatrix}$$

of rank 3, and μ as above.

In view of applications to Tikhonov-Fenichel reduction via Theorem 1, there is particular interest in situations where the conclusion of Lemma 1, part (c) holds. Some notable results on this question are known, such as the following Deficiency Zero Theorem by Horn and Jackson [23], and Feinberg [13].

Proposition 3. *Assume that a reaction network has deficiency zero, and is weakly reversible. Let a decomposition as in Lemma 1(a) be given. Then every positive SCC contains precisely one stationary point, which is locally asymptotically stable. The stationary points in ${\mathbb{R}^*_+}^n$ form a submanifold of dimension $n - q$, and $\mathbb{R}^n = \operatorname{Ker} Df(x) \oplus \operatorname{Im} Df(x)$ for each of these stationary points.*

Proof. For the first and second assertion see [13], Thm. 4.1, the third holds according to [13], Remark 4.3, and the last one follows from [13], Thm. 4.3 together with Remark 4. □

Remark 7. There are several generalizations and specializations of this result.

(a) The Deficiency One Theorem (Feinberg [13], Thm. 4.2, is based on the following hypotheses: Deficiency ≤ 1 for each linkage class; the total deficiency equals the sum of the deficiencies for the linkage classes; every linkage class contains just one terminal strong-linkage class. Then, assuming that there exists a stationary point in ${\mathbb{R}_+^*}^n$, the second conclusion of Proposition 3 still holds true.

(b) Bothe [6], Thm. 1, is based on the (strong) assumption that the network is reversible, and that the stoichiometric vectors associated with pairs of forward-reverse reactions form a linearly independent set. Under these conditions (which imply deficiency zero) there is a globally asymptotically stable stationary point in each SCC. Moreover the asymptotic stability is locally uniform (when the stationary point runs through varying SCC), in the sense that there exists a Lyapunov function, and a locally uniform estimate for its Lie derivative. (This property is not stated explicitly in [6], but follows from the inequality on p. 33, last line.)

(c) If a stationary point x_0 in a positive SCC is linearly asymptotically stable in its compatibility class, then the stationary points locally form a manifold of dimension $n - q$, and one has the direct sum decomposition $\mathbb{R}^n = \operatorname{Ker} Df(x) \oplus \operatorname{Im} Df(x)$ for every stationary point. See Remark 4 and [19], Prop. 8.3.

(d) Schauer and Heinrich [34], Section 4, discuss the condition (at a stationary point x_0)

$$f(x_0) = 0 \text{ and } \operatorname{rank} S\, D\theta(x_0) = \operatorname{rank} S \left(\Leftrightarrow \operatorname{rank} \widetilde{P}\, D\widetilde{\mu}(x_0) = \operatorname{rank} \widetilde{P} \right).$$

They note that this condition is sufficient to ensure the existence of a local $(n - q)$-dimensional submanifold of stationary points; but (as Example 4 illustrates) there is no direct sum decomposition in general. See also the *rank condition* in Lee and Othmer [28], p. 407 on this. (Schauer and Heinrich moreover assert that their rank condition is satisfied whenever all reactions in the network are reversible.)

3.2 Reduction via stoichiometry

In this section, we discuss a system of reaction equations with a separation into slow and fast reactions. The focus is on systems which admit a Tikhonov-Fenichel reduction through the stoichiometric decomposition of the fast part. Thus we have

$$\dot{x} = h^{(0)}(x) + \varepsilon h^{(1)}(x), \quad x \in \mathbb{R}_+^n, \tag{16}$$

and focus on decompositions

$$h^{(0)}(x) = S\, \theta(x) \tag{17}$$

with a stoichiometric matrix S of rank $q < n$, refined according to Lemma 1(a), thus

$$h^{(0)}(x) = \widehat{P}\,\widehat{\mu}(x) \tag{18}$$

with a constant matrix $\widehat{P}$.

Proposition 4. *Let system* (16) *be given, with decompositions* (17) *and* (18) *for the fast part, and let x_0 be a nonnegative stationary point of $h^{(0)}$. Then the following hold.*

(a) If x_0 is isolated in its SCC, and $D\widehat{\mu}(x_0)\,\widehat{P}(x_0)$ is invertible then there exists a formal Tikhonov-Fenichel reduction of (16) *in the sense of Remark 3. In particular such a formal reduction exists whenever $x_0 \in {\mathbb{R}^*_+}^n$ and the hypotheses of Feinberg's deficiency-one theorem (see Remark 7) are satisfied for $h^{(0)}$.*

(b) If the hypotheses of (a) are satisfied then the reduced equation may be determined directly from the decomposition (17)*: For x near x_0 the linear equation*

$$D\theta(x)S\alpha = D\theta(x)h^{(1)}(x), \text{ for } \alpha \in \mathbb{R}(x)^n$$

has a solution $\alpha^*(x) \in \mathbb{R}(x)^n$, which gives the reduced system

$$x' = h^{(1)}(x) - S\alpha^*(x). \tag{19}$$

(c) If the reaction network underlying $h^{(0)}$ has deficiency zero, and the uniformity condition for asymptotic stability from Verhulst [40], Thm. 8.1b holds for all stationary points near x_0 then the convergence property holds for the formal Tikhonov-Fenichel reduction. In particular this holds whenever all nonzero eigenvalues of $Dh^{(0)}(x_0)$ have negative real part, and also given the conditions stated by Bothe [6] (see Remark 7).

Proof. Parts (a) and (c) are immediate consequences of the statements in Proposition 3 and Remark 7. For part (b), the observation

$$\operatorname{rank} Dh^{(0)}(x_0) = \operatorname{rank} S\,D\theta(x_0) = \operatorname{rank} S$$

shows that $\operatorname{Ker} D\theta(x_0) \cap \operatorname{Im} S = \{0\}$, and then (by inclusion and equal dimensions)

$$\operatorname{Ker} Dh^{(0)}(x_0) = \operatorname{Ker} D\theta(x_0), \quad \operatorname{Im} Dh^{(0)}(x_0) = \operatorname{Im} S.$$

For $y \in \mathbb{R}^n$ we thus have a kernel-image decomposition

$$y = z + S\alpha \Rightarrow D\theta(x_0)y = D\theta(x_0)S\alpha;$$

in particular the linear equation stated in (b) admits a solution α^*, and the assertion follows.

□

Remark 8. The uniformity condition mentioned in Verhulst [40], Ch. 8 is stated in detail in Hoppensteadt [22], under the name of Condition VI. It may actually be true that in the analytic setting the uniformity condition is always satisfied, but there seems to be no simple proof. Due to Proposition 4, Bothe's [6] Theorem 2 can be proved directly via Tikhonov.

Example 6 (Suicide kinetics, again)**.** We discuss suicide kinetics with $k_1 = \varepsilon\kappa_1$ as small parameter. Using the results from Example 5 and discarding the equations for p and e_i, we have

$$h^{(0)} = \begin{pmatrix} -1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -(k_3+k_4) \end{pmatrix} \cdot \begin{pmatrix} k_{-1}x \\ k_2 x \\ y \end{pmatrix}, \quad h^{(1)} = k_1 \begin{pmatrix} -es \\ -es \\ es \\ 0 \end{pmatrix}. \tag{20}$$

The variety of the fast term $\mathcal{V}(\mu) = \{(e, s, 0, 0)^T\}$ defines the slow manifold. We proceed with

$$\begin{pmatrix} k_{-1}x \\ k_2 x \\ y \end{pmatrix} = \begin{pmatrix} k_{-1} & 0 \\ k_2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

and thus get the appropriate decomposition

$$h^{(0)} = \begin{pmatrix} -k_{-1} & 0 \\ k_{-1} & 0 \\ k_{-1}-k_2 & 0 \\ 0 & -(k_3+k_4) \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} =: P \cdot \mu$$

in accordance with Lemma 1. Furthermore one finds

$$D\mu\, P = \begin{pmatrix} k_{-1}-k_2 & 0 \\ 0 & -(k_3+k_4) \end{pmatrix}$$

Note that one must require $k_{-1} \neq k_2$ to ensure invertibility of $D\mu\, P$. The projection matrix turns out to be

$$\begin{pmatrix} 1 & 0 & \frac{k_{-1}}{k_{-1}-k_2} & 0 \\ 0 & 1 & -\frac{k_{-1}}{k_{-1}-k_2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and finally the reduced system is

$$\begin{aligned} \dot{e} &= -\tfrac{k_1 k_2}{k_{-1}-k_2} es \\ \dot{s} &= -\tfrac{k_1(k_2-2k_{-1})}{k_{-1}-k_2} es, \end{aligned} \tag{21}$$

with an elementary solution.

4 Application: Maltose transport

In this section we discuss a Tikhonov-Fenichel reduction to a one-dimensional variety which does not seem to allow an explicit parameterization. Nevertheless we are able to analyze the limiting behavior of the reduced system, since the qualitative behavior of vector fields on one-dimensional submanifolds (and by extension on varieties) is well-understood. Thus the example also illustrates how reduction to a nontrivial variety will provide useful information for further analysis.

Stiefenhofer [37] discusses a transport mechanism through a biomembrane, with a mechanism based on selective permeability. In order to pass through the cell membrane, a maltose molecule X first reacts with a so-called binding protein Z to a complex Y_1. The latter reacts with the membrane-bound receptor R, forming a complex Y_2, which subsequently degrades, thus releasing maltose into the cell. This last process is modelled by reaction E_1^*, where X_i stands for maltose in the interior of the cell. In addition, Stiefenhofer assumes a direct reaction E_4^* between the binding protein and the mebrane receptors. Altogether, the transport mechanism is modelled by the network

$$\begin{array}{llll} E_1^*: & Y_2 \overset{k_1}{\rightharpoonup} R+Z+X_i & E_2^*: & Z+X \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} Y_1 \\ E_3^*: & Y_1+R \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} Y_2 & E_4^*: & Z+R \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} Y_3. \end{array}$$

The corresponding reaction rates are

$$\begin{array}{llll} E_1 := & -y_2 & E_2 := & y_1 - zx \\ E_3 := & y_2 - y_1 r & E_4 := & y_3 - zr \end{array}$$

and the reaction equations (with ξ denoting the concentration of X_i) thus are

$$\begin{array}{rcccccccc} \dot{x} &=& & & E_2 & & & & \\ \dot{z} &=-& \varepsilon E_1 &+& E_2 & & & + & E_4 \\ \dot{r} &=-& \varepsilon E_1 & & & + & E_3 & + & E_4 \\ \dot{\xi} &=-& \varepsilon E_1 & & & & & & \\ \dot{y}_1 &=& & - & E_2 & + & E_3 & & \\ \dot{y}_2 &=& \varepsilon E_1 & & & - & E_3 & & \\ \dot{y}_3 &=& & & & & & - & E_4 \end{array} \tag{22}$$

From stoichiometry one has linear first integrals

$$z + y_1 + y_2 + y_3, \quad r + y_2 + y_3, \quad x + \xi + y_1 + y_2.$$

With initial conditions $x(0) = x_0 > 0$, $z(0) = z_0 > 0$, $r(0) = r_0 > 0$, $\xi(0) = \xi_0 > 0$ and $y_1(0) = y_2(0) = y_3(0) = 0$ we obtain a four-dimensional system for $(\xi, y_1, y_2, y_3)^T$, upon replacing

$$z = z_0 - (z + y_1 + y_2 + y_3), \quad r = r_0 - (y_2 + y_3), \quad x = x_0 + \xi_0 - (\xi + y_1 + y_2).$$

We note that the compact set

$$L := \{(\xi, y_1, y_2, y_3)^T \in \mathbb{R}^4_+;\ y_1+y_2+y_3 \le z_0, y_2+y_3 \le r_0, \xi+y_1+y_2 \le \xi_0+x_0\}$$

is positively invariant for this four-dimensional system.
According to [37], the release of maltose into the cell is slow compared to the other reactions, i. e. k_1 is a small parameter. The fast and slow terms are therefore given by

$$h^{(0)} = \begin{pmatrix} 0 \\ -E_2+E_3 \\ -E_3 \\ -E_4 \end{pmatrix}, \quad h^{(1)} = \begin{pmatrix} -E_1 \\ 0 \\ E_1 \\ 0 \end{pmatrix}.$$

For this system, Stiefenhofer [37] discussed the initial phase of the process and obtained a starting value on the slow manifold. In the present paper we investigate the quasi-steady state phase.
The reduction works for arbitrary rate constants, but (following [37]) to keep the output size manageable we fix the rate constants $k_2 = k_{-2} = k_3 = k_{-3} = k_4 = k_{-4} = 1$ from now on. We get a matrix decomposition $h^{(0)} = P \cdot \mu$ with

$$\mu = \begin{pmatrix} E_2 \\ E_3 \\ E_4 \end{pmatrix} = \begin{pmatrix} y_1 - (z_0 - (y_1+y_2+y_3))(x_0+\xi_0-\xi-(y_2+y_1)) \\ y_2 - y_1(r_0-(y_2+y_3)) \\ y_3 - (z_0-(y_1+y_2+y_3))(r_0-(y_2+y_3)) \end{pmatrix}$$

and

$$P = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A formal reduction exists if and only if the matrix

$$D\mu \cdot P = \begin{pmatrix} \xi-\xi_0+2(y_1+y_2)+y_3-(x_0+z_0+1) & 1 & \xi-\xi_0+y_1+y_2-x_0 \\ -(y_2+y_3)+r_0 & -y_1+y_2+y_3-(r_0+1) & -y_1 \\ y_2+y_3-r_0 & y_1+y_2+y_3-z_0 & y_1+2y_2+2y_3-(r_0+z_0+1) \end{pmatrix}$$

is invertible. Setting

$$b = D\mu \cdot h^{(1)} = \begin{pmatrix} y_2(\xi-\xi_0+y_1+y_2-x_0) \\ -y_2(y_1+1) \\ y_2(y_1+2(y_2+y_3)-(r_0+z_0)) \end{pmatrix},$$

then

$$\alpha = \frac{1}{n}\begin{pmatrix} \xi-\xi_0+y_1+y_2-(x_0+1) \\ \xi-\xi_0+2(y_1+y_2)+y_3-(x_0+z_0+1) \\ y_2(y_1+y_2+y_3-z_0)(y_2+y_3-r_0) \end{pmatrix}$$

with polynomial denominator

$$n = \xi_0-\xi+(y_1+y_2+y_3-z_0)(y_2+y_3-r_0-1)-(y_1+y_2)+1+x_0$$

solves the linear equation

$$(D\mu P)\cdot\alpha = b.$$

(Note that $n > 0$, due to initial values and first integrals.) As remarked in Proposition 4(b) the reduced vector field is given by $h^{(1)} - P\alpha$, explicitly

$$\begin{aligned}
\dot\xi &= y_2\\
\dot y_1 &= \frac{y_2(y_1+y_2+y_3-z_0)}{n(\xi,y_1,y_2,y_3)}\\
\dot y_2 &= -y_2 - \frac{y_2(\xi-\xi_0+2(y_1+y_2)+y_3-(x_0+z_0+1))}{n(\xi,y_1,y_2,y_3)}\\
\dot y_3 &= \frac{y_2((y_2+y_3)(y_1+y_2+y_3-r_0-z_0)+r_0(z_0-y_1))}{n(\xi,y_1,y_2,y_3)}
\end{aligned} \tag{23}$$

on the one-dimensional slow manifold $Y := \mathcal{V}(\mu)\setminus\mathcal{V}(\det D\mu P)$. It seems impossible to determine an explicit parameterization of this algebraic curve, but we will be able to give a complete qualitative analysis. We first recall a few general facts.

Remark 9. The behavior of (polynomial or rational) vector fields on one-dimensional varieties is rather easy to understand. The singular points of such a variety (which are finite in number) form an invariant set, thus are stationary. The complement of the singular set is a finite union of submanifolds (without boundary), and each connected component is diffeomorphic either to $\mathbb{R}$ or to the circle $\mathbb{S}^1$ (see e.g. Milnor [30], Appendix). The qualitative behavior of differential equations on $\mathbb{R}$ is well-understood: Nonstationary trajectories are unbounded or have stationary limit points (in either direction). Likewise, nonstationary trajectories on the circle connect stationary points if there are any (which then are limit points), or correspond to periodic solutions.

Proposition 5. *(a) The intersection $K := L \cap Y$ is positively invariant for (23). The determinant of $D\mu P$ is nonzero on L, hence a formal Tikhonov-Fenichel reduction exists on L.*

(b) Y is a reducible variety, with two irreducible components (in the Zariski topology) and there are no singular points in K. There are two stationary points on Y, viz.

$$\begin{aligned}
s_1 &:= \left(\xi_0+x_0,\ 0,\ 0,\ \tfrac{r_0+z_0+1}{2} + \sqrt{\tfrac{(r_0+z_0+1)^2}{4} - r_0 z_0}\right)^T,\\
s_2 &:= \left(\xi_0+x_0,\ 0,\ 0,\ \tfrac{r_0+z_0+1}{2} - \sqrt{\tfrac{(r_0+z_0+1)^2}{4} - r_0 z_0}\right)^T.
\end{aligned}$$

Only s_2 lies in K.

(c) There is no closed connected component of Y (in the norm topology) that intersects L. Only one connected component of Y has nonempty intersection with L, and the intersection contains s_2.

(d) The stationary point s_2 is globally asymptotically stable on K. Concerning the linearization of the restriction of (23) to Y, the eigenvalue (which governs the approach to the stationary point) is

$$\lambda := \frac{s_{2,3} - z_0}{(s_{2,3} - r_0 - 1)(s_{2,3} - z_0) + 1},$$

with $s_{2,3}$ the y_3-component of s_2. An eigenvector is given by $(1, \lambda, \lambda, \lambda)^T$.

Proof. The positive invariance of K for (23) follows from the positive invariance of L for the four-dimensional system and the reduction formula. Moreover

$$\begin{aligned}\det\,(D\mu P) = (2(y_3 + y_2) - z_0 - r_0 - 1)((\xi_0 + x_0 - \xi - y_1 - y_2) \\ +(z_0 - y_1 - y_2 - y_3)) + (1 + (r_0 - y_2 - y_3)(z_0 - y_1 - y_2 - y_3))\end{aligned}$$

is > 0 on L by inspection. For instance the term

$$2(y_3 + y_2) - z_0 - r_0 - 1 = (y_2 + y_3 - z_0) + (y_2 + y_3 - r_0) - 1$$

is negative on L, and the other terms can be analyzed similarly. Thus (a) is proven.

To prove the first assertion of (b), we use SINGULAR [10] to compute a primary decomposition of the vanishing ideal $\mathcal{I}(\mathcal{V}(\mu))$ and take radicals. (See Decker and Lossen [11], Ch. 7 for background.) Thus we obtain a decompostion of $\mathcal{V}(\mu)$ into two irreducible components $\mathcal{V}(\mu) = W_1 \cup W_2$. As a practical matter we let

$$u = \sqrt{\frac{(r_0 + z_0 + 1)^2}{4} - r_0 z_0},$$

take $\mathbb{Q}[u]$ as a base ring and add the minimum polynomial of u to the ideal generators. The ideal $\mathcal{I}(W_1)$ is generated by

$$\begin{aligned}
\omega_1 &= u^2 - (r_0 + z_0 + 1)u + r_0 z_0, \\
\omega_2 &= y_2 + y_3 - u, \\
\omega_3 &= r_0(y_1 + y_2) - y_3 u + (r_0 + z_0 + 1)y_3 - r_0 z_0, \\
\omega_4 &= r_0 z_0 \xi y_3 + z_0 y_3^2 u - z_0(r_0 + z_0 + 1)y_3^2 + (x_0 + \xi_0 - z_0 + 1)z u^2 \\
&\quad +((z_0 - 1)(r_0 + 1) - (x_0 + \xi_0)(r_0 + z_0 + 1))y_3 u \\
&\quad +((r_0 + z_0 + 1)^2 + r_0 z_0)u - r_0 z_0(r_0 + z_0 + 1) - (r_0 + z_0 + 1)u^2
\end{aligned}$$

over $\mathbb{Q}[u]$ (respectively over $\mathbb{Q}$, upon substitution for u). Generators of $\mathcal{I}(W_2)$ are

$$\begin{aligned}
\omega_5 &= u^2 - (r_0 + z_0 + 1)u + r_0 z_0, \\
\omega_6 &= y_2 + y_3 + u - (r_0 + z_0 + 1), \\
\omega_7 &= r_0(y_1 + y_2) + y_3 u - r_0 z_0, \\
\omega_8 &= r_0 z_0 \xi y_3 - z_0 y_3^2 u + (x_0 + \xi_0 - z_0 + 1)z u^2 + (-(x_0 + \xi_0) \cdot \\
&\quad (r_0 + z_0 + 1) + (z_0 - 1)(r_0 + 1))y_3 u + ((r_0 + z_0 + 1)^2 - r_0 z_0)u \\
&\quad -(r_0 + z_0 + 1)u^2.
\end{aligned}$$

By straightforward computation one finds the stationary points on $\mathcal{V}(\mu)$, namely

$$\begin{aligned} s_1 &:= \left(\xi_0 + x_0,\ 0,\ 0,\ \tfrac{r_0+z_0+1}{2} + \sqrt{\tfrac{(r_0+z_0+1)^2}{4} - r_0 z_0}\right)^T, \\ s_2 &:= \left(\xi_0 + x_0,\ 0,\ 0,\ \tfrac{r_0+z_0+1}{2} - \sqrt{\tfrac{(r_0+z_0+1)^2}{4} - r_0 z_0}\right)^T. \end{aligned}$$

One checks $s_1 \in W_1$ and $s_2 \in W_2$ by substitution into the ideal generators. On L one has $y_2 + y_3 \leq (r_0 + z_0)/2$, and this shows that $s_1 \notin K$. Let g be the right-hand side of the reduced equation. The linearization of (23) in s_2 reads

$$Dg(s_2) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & \lambda & 0 \end{pmatrix}.$$

This matrix has eigenvalue 0 with multiplicity 3 and one nontrivial eigenvalue $\lambda < 0$. The nonzero eigenvalue corresponds to the tangent space of Y (see e.g. the arguments on NFIS in Bibikov [2]), hence the stationary point s_2 is linearly asymptotically stable for the restriction to Y.
There remains to prove that $s_2 \in K$ and that K contains no closed connected component. Assume that such a closed component exists. Then it cannot contain $s_1 \notin K$, and also it cannot contain s_2, since s_2 cannot be an α-limit point. Therefore nontrivial periodic solutions must exist. But inspecting the first entry of (23) shows (by monotonicity) that a periodic solution must have y_2-entry zero, and thus be stationary; a contradiction.
Since the ω-limit set of any point in K is nonempty, Remark 9 shows that K must contain a stationary point (thus necessarily s_2) and this stationary point is the ω-limit point for all solutions in K.
Thus all claims are proven. □

There remains the legitimate question to what extent this Proposition holds for general parameters k_i, rather than the special ones chosen. Part (a) remains true (with appropriately modified definitions of L and K), as does the assertion that there is no nonconstant periodic solution, since the monotonicity argument remains valid. On the other hand, the number of irreducible components and the number and properties of stationary points may vary, in principle; this would require further study by algebraic means.

A Appendix

A.1 Some algebra

We give a brief account of some notions and results from classical commutative algebra and algebraic geometry. In our context these are mostly relevant for computational and algorithmic purposes. A more detailed (application-oriented) presentation is given in the monograph by Cox, Little, O'Shea [9];

in proofs below we will refer to some special results stated in Shafarevich [36]. A very good short introduction to commutative algebra and algebraic geometry is contained in Humphreys [24], Ch. I; much of what we need is already contained in Subsections 1.1 to 1.3 of this monograph. We let $\mathbb{K}$ stand for $\mathbb{R}$ or the complex numbers $\mathbb{C}$.

1. With $\mathbb{K}[x_1, \ldots, x_n]$ we denote the polynomial ring in n variables; we will regard a polynomial as a map from $\mathbb{K}^n$ to $\mathbb{K}$. A subset $Y \subseteq \mathbb{K}^n$ will be called *Zariski-closed*, or an *affine algebraic variety* if there exist finitely many polynomials $\phi_1, \ldots, \phi_r$ such that Y is the set of common zeros of these polynomials in $\mathbb{K}^n$; we will write $Y = \mathcal{V}(\phi_1, \ldots, \phi_r)$. Rather than considering polynomials $\phi_1, \ldots, \phi_r$ one looks at the ideal $\mathcal{I} = \langle \phi_1, \ldots, \phi_r \rangle$ they generate; note that Y is the common zero set of all the elements of $\mathcal{I}$. The complement of a Zariski-closed set in $\mathbb{K}^n$ is called *Zariski-open* (this is an open and dense set in the norm topology, unless empty), and we transfer this notion to Zariski-open subsets of affine varieties in the obvious way.

2. There is one particular feature of the Zariski topology: One calls a Zariski-closed set Y *reducible* if there are Zariski-closed sets Y_1, $Y_2 \subset Y$ with $Y_i \neq Y$, $i = 1, 2$ but $Y_1 \cup Y_2 = Y$, and *irreducible* otherwise. Every Zariki-closed set is a finite union of irreducible components: $Y = Y_1 \cup \cdots \cup Y_m$, with no Y_i a subset of another Y_j, and this representation is unique up to ordering.

3. With $\mathbb{K}(x_1, \ldots, x_n)$ we denote the field of rational functions in n variables; a rational function may be seen as a map from a Zariski-open subset U of $\mathbb{K}^n$ (those points where the denominator is nonzero) to $\mathbb{K}$. One may extend the notion of rational function to irreducible varieties by restriction, but note that the variety should not be contained in the zero set of the denominator. If Y is irreducible and $a \in Y$ then the local ring of a (denoted by $\mathcal{O}_a$ or $\mathcal{O}_{a,Y}$) is defined as the set of all rational functions that can be represented as a quotient of polynomials with nonzero denominator at a. (One then says that such functions are regular at a.)

4. Given $Y = \mathcal{V}(\phi_1, \ldots, \phi_r)$ and $a \in Y$, the *tangent space* of Y in a is defined as
$$T_a(Y) := \{z \in \mathbb{K}^n;\, D\phi_1(a)z = \cdots D\phi_r(a)z = 0\}\,,$$
similar to the definition for submanifolds of $\mathbb{K}^n$. One can show that this notion does not depend on the specific choice of the ϕ_i. A point $a \in Y$ is called *simple* if (i) a is contained in only one irreducible component Y_i of Y, and (ii) the dimension of $T_a(Y)$ is not greater than the dimension of $T_b(Y)$, for any $b \in Y_i$. (The dimension of $T_a(Y)$ is also equal to the dimension of the variety Y_i.) The simple points of Y_i form a Zariski-open and dense subset of Y_i, which is also a submanifold of $\mathbb{K}^n$ in the usual sense. This observation also implies that any affine algebraic variety, as well as any Zariski-open subset of such a variety, is a finite union of submanifolds.

A.2 Proof of Theorem 1

We first state a lemma which essentially says that a $n-r$–dimensional subvariety of $\mathbb{K}^n$ can locally, near a simple point, be represented as the common zero set of r rational functions. A proof is given in Shafarevich [36], Ch. II, §2.3 (using special properties of $\mathbb{K}$), and also for a more general setting in [36], Ch. II, §3, Thm. 5, using special properties of the local ring. (The proof of Thm. 5 is given for an algebraically closed base field, but in case $\mathbb{K} = \mathbb{R}$ one obtains the assertion by taking real parts. The more general statement from Thm. 5 becomes relevant when one considers successive reductions, thus also reductions starting on varieties.)

Lemma 2. *Let $\mu_1, \ldots, \mu_m \in \mathbb{K}(x_1, \ldots, x_n)$, $Y = \mathcal{V}(\mu_1, \ldots, \mu_m)$, and $a \in Y$ a simple point. Let $\widetilde{Y} \subseteq Y$ the irreducible component which contains a, with $\dim \widetilde{Y} = n - r$. Moreover assume (w.l.o.g., up to relabeling) that*

$$\operatorname{rank} \begin{pmatrix} D\mu_1(a) \\ \vdots \\ D\mu_r(a) \end{pmatrix} = r.$$

Then for any $\eta \in \mathbb{K}(x_1, \ldots, x_n)$ which (is regular and) vanishes on $\widetilde{Y}$, there exist $\vartheta_1, \ldots, \vartheta_r \in \mathbb{K}(x_1, \ldots, x_n)$, regular at a, such that

$$\eta = \vartheta_1 \mu_1 + \cdots + \vartheta_r \mu_r.$$

Proof of the theorem. (a) The first (as well as the last)assertion is a direct consequence of Lemma 2, taking the entries of $h^{(0)}$ to be $\mu_1, \ldots, \mu_n$, assuming $\mu_{i_1}, \ldots, \mu_{i_r}$ to be independent at a and applying the statement of the Lemma to each μ_j. The irreducible component $\widetilde{Y}$ of $\mathcal{V}(h^{(0)})$ which contains a has dimension $n - r$. Thus the rank of $Dh^{(0)}(x)$ is equal to r in some Zariski neighborhood of a in $\mathcal{V}(h^{(0)})$, since smaller rank is characterized by the vanishing of certain minors.

(b) A step-by-step derivation of (8) was given in [19]. Here we present a shorter version.
There is a Zariski-open neighborhood U_a of a in $\mathbb{R}^n$ such that

$$\mathbb{R}^n = \operatorname{Ker}\, Dh^{(0)}(x) \oplus \operatorname{Im}\, Dh^{(0)}(x)$$

for all $x \in \mathcal{U}_a := U_a \cap \widetilde{Y}$, since the kernel must have dimension $n-r = \dim \widetilde{Y}$. Since $P(x)$ has full rank, we get

$$\operatorname{Ker}\, Dh^{(0)}(x) = \operatorname{Ker}\, D\mu(x) \quad \text{and} \quad \operatorname{Im}\, Dh^{(0)}(x) = \operatorname{Im}\, P(x)$$

and furthermore

$$Dh^{(0)}(x) = P(x)\, D\mu(x)$$

for all $x \in \mathcal{U}_a$. Moreover by Remark 4, $A(x) := D\mu(x)\,P(x)$ is invertible for all $x \in \mathcal{U}_a$.
Since

$$\begin{array}{rcl} & D\mu(x)\left(Id - P(x)A(x)^{-1}D\mu(x)\right)\,h^{(1)}(x) & \\ = & \left(D\mu(x) - A(x)A(x)^{-1}D\mu(x)\right)\,h^{(1)}(x) & = \quad 0, \end{array}$$

every component of μ is a first integral of (8). The invariance assertion follows from part (a).

(c) Now let

$$v = v_0 + v_1 \in \mathbb{R}^n; \quad v_0 \in \operatorname{Ker} Dh^{(0)}(x), \quad v_1 = P(x)w \in \operatorname{Im} Dh^{(0)}(x).$$

Then

$$P(x)A(x)^{-1}D\mu(x)\,(v_0 + v_1) = P(x)A(x)^{-1}D\mu(x)P(x)w = P(x)w = v_1,$$

whence $Id - P(x)A(x)^{-1}D\mu(x)$ projects any vector to its kernel component with repect to the kernel-image decomposition. According to [32], Lemma 2.4 and Proposition 2.5, the reduced system for (2) is obtained as the kernel component of $h^{(1)}(x)$ in the kernel-image decomposition with respect to $Dh^{(0)}(x)$. This finishes the proof.

□

A.3 Algorithmic decomposition

The decomposition introduced in Lemma 2 can be carried out constructively with the help of standard bases; see Decker and Lossen [11], in particular Lecture 9, for a general introduction and details concerning the algorithms. Here we give a short outline of the procedure, for the reader's convenience. Thus assume the situation in Lemma 2 is given. Regarding the local ring $\mathcal{O}_a$, the lemma states that

$$I := \langle \mu_1, \ldots, \mu_r \rangle$$

is the vanishing ideal ideal of $\widetilde{Y}$. Given $\eta \in I$, one obtains the ϑ_j in three steps:

1. Given a local monomial order, denote by $L(\gamma)$ the leading term of a monomial. The first step is to complete $M := \{\mu_1, \ldots, \mu_r\}$ to a standard basis of I. To do so, given a generating set $q_1, \ldots, q_\ell$ of I, one computes all S-polynomials

$$s_{i,j} := S(q_i, q_j) = \frac{L(q_j)}{\gcd(L(q_j), L(q_i))} q_i - \frac{L(q_i)}{\gcd(L(q_i), L(q_j))} q_j \in \mathcal{O}_a,$$

$1 \le i, j \le \ell$, augments the generating set by the $s_{i,j} \notin \{q_1, \ldots, q_\ell\}$, and continues the process with the augmented set. As shown in [11], this process terminates; thus after finitely many steps one obtains a standard basis from $\mu_1, \ldots, \mu_r$.

2. Given any set $\{\phi_1, \ldots, \phi_k\} \subset I$ and a nonzero $\eta \in \mathcal{O}_a$, Mora's division algorithm (see [11], Thm. 9.19) yields ρ and $\gamma_1, \ldots, \gamma_k \in \mathcal{O}_a$, such that

$$\eta = \sum_{i=1}^{k} \gamma_i \phi_i + \rho$$

and

- (DIV 1): $L(\eta) \geq L(\gamma_i \phi_i)$, $1 \leq i \leq k$ (unless $\gamma_i \phi_i = 0$).
- (DIV 2): $L(\rho)$ is not divisible by any of $L(\phi_i)$, $1 \leq i \leq k$ unless $\rho = 0$.

For a standard basis $\{\phi_1, \ldots, \phi_k\}$ the remainder ρ vanishes if and only if $\eta \in I$.

3. Now consider a standard basis

$$\phi_i = \begin{cases} \mu_i, & 1 \leq i \leq r, \\ \sigma_i, & r+1 \leq i \leq k, \end{cases}$$

of I which is obtained from $\mu_1, \ldots, \mu_r$ by successively adjoining S-polynomials $\sigma_{r+1}, \ldots, \sigma_k$. For $\eta \in I$ we obtain a representation $\eta = \sum_{i=1}^{r} \gamma_i \phi_i$. Since ϕ_i can be expressed as a linear combination of $\phi_1, \ldots, \phi_{i-1}$ as long as $i > r$, succcessive substitution yields a representation

$$\eta = \sum_{i=1}^{r} \vartheta_i \mu_i$$

with $\vartheta_i \in \mathcal{O}_a$ for $1 \leq i \leq r$.

There is an implementation of Mora's algorithm in the computer algebra system SINGULAR; see [10]. Thus we see, as stated earlier, that the reduction of rational systems can be obtained in an algorithmic fashion.

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