On a decomposition of motions and model reduction

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Abstract. In this work a concept of Singularly Perturbed Vector Fields (SPVF) (proposed in previous authors' papers) is further applied to practical problem of developing a robust numerical tool for model reduction. The paper is focused on the construction of an algorithm which allows a linear transformation of dimensional combustion models (written as systems of ODEs) to an explicitly decomposed form that can be treated by the standard theory of Singular Perturbed Systems (SPS), which allows the reduction of a system dimension by the standard decomposition to "fast" and "slow" subsystems and by using slow the invariant(integral) manifolds' concept. As a result, the algorithm can essentially simplify numerical aspects of simulation of complex processes taking place in reacting flows.

1. Introduction

Recently, a problem of the modelling of reacting flows has become important due to significant progress in hardware and software development. New powerful workstations, computing clusters, and supercomputers, together with variety of software packages of numerical integration, allow detailed treatment of complex processes taking place in the reacting flows [1]. Novel software packages simplify significantly not only the actual integration part (CHEMKIN, COSILAB etc.), but the development stage of the mathematical model has also become almost automatic (see e.g. [2–6]).

As a result more and more detailed kinetics mechanisms have been designed to improve chemical reaction models for a better understanding of the governing processes and peculiarities of the reacting flows. Furthermore, in order to increase efficiency and to advance the design of industrial, engineering and technological tools (such as internal combustion engines, gas turbines, power plants etc.) as well as methods of organic and inorganic synthesis (biotechnology, structural molecular design etc.) more sophisticated detailed models have to be developed, simulated and analyzed. This leads to an enormous growth of a system of governing differential equations in both dimension and complexity aspects. Therefore, it is of a great interest to have a suitable tool for automatic model reduction without significant damage to the overall qualitative and quantitative properties of the reduced model by comparison with the original one [7, 8].

A large number of practical systems involve subprocesses with essentially different time scales. The discrepancy in time scales permits decomposition of motions of the original models and, consequently, allows a reduction in the original system dimension and its complexity. A number of analytical and numerical methods based on the multi-scale nature of such system was proposed (see e.g. [9–16]). The main problem with such approaches is in the implicit nature of the
multi-scale structure, namely, for complex realistic models this structure is "hidden" in the original mathematical model. Sometimes (for comparatively simple models) such subdivision can be explicitly delineated using physical or engineering knowledge about the processes under investigation, but, in the general case, the transition from the original system with the "hidden" multi-scale structure to its explicit representation as a standard singularly perturbed system (SPS) is not a trivial task. It requires a deep understanding of the mathematical model’s properties and also a large amount of time (human resources) to find a particular decomposed form, which, in turn, can vary from one parametric region (of the system’s parameters) to another.

Thus, an automatic procedure for model reduction is required, which is based on the assumption of existence of a multi-scales structure of the original system of governing equations. Under such assumption the only problem which has to be solved is the automatic transformation of the original system into the standard SPS form. In the case that such transformation is found the obtained explicit SPS can be treated by the very powerful machinery of the standard SPS theory for reduction/decomposition purposes (see e.g. [17–22] for more detail).

In this paper we extend further the coordinate free concept of singularly perturbed systems (SPS), the so-called singularly perturbed vector fields (SPVF, see e.g. [23] for definitions and for more detail) and apply this machinery for designing an algorithm that allows such transformation of the original system into suitable SPS form with its subsequent reduction. The main purpose of this stage of the study and the problems which have to be solved are the simplicity (from implementation point of view) and robustness of the designed algorithm of the transformation. Moreover, properties like robustness of the procedure and consistency of the reduced model to the detailed one are the focus of the current results.

For illustration and verification several 2D test models as well as a 3D enzyme interaction model are considered. The structure of the decomposed system dynamics is compared with the detailed one by a phase space analysis. The comparison shows that the overall complexity of the novel method reduces, whereas new properties of the decomposed structure (fast manifolds, global dimension and stability analysis etc.) become available due to the suggested method.

The paper is organized as follows. First, we present a brief outline of the coordinate free concept which is a core of the suggested algorithm. It is also serves as a theoretical basis for the reduction itself and consists of technical tools and notations useful for presenting the approach. Second, after all necessary definitions have been introduced, the so-called linearization procedure is presented together with properties of typical kinetics models that allow the decomposition. Then, some important problems of the suggested earlier realization of the Global Quasi Linearization (GQL) are discussed and overcome by using suitable modification of the GQL and by a new kind of sorting procedure. The criteria for choice of the corresponding scalar invariant for GQL are obtained. They are founded on some geometrical invariants of the original vector fields considered in the domain of interest in the system’s state or phase space. In the final sections, properties of the algorithm are discussed and verified on a number of model systems.

2. General Notion of Singularly Perturbed Vector Fields

We begin an introduction to the general framework of Singularly Perturbed Vector Fields (SPVF) with an informal definition that delineates the geometrical essence of the approach and serves as a motivation to the formal concept. The vector field \( F(x, \varepsilon) \) is defined as a SPVF in a domain \( \Omega \) of the Euclidian space \( \mathbb{R}^n \) if it depends on a small parameter \( \varepsilon \geq 0 \) such that the limiting vector field \( F(x,0) \) belongs to a fast subspace \( L_f(x) \) of smaller dimension - \( \dim L_f(x) < n \) which, \textit{a priori}, fixed for any point \( x \). This property of degeneration of the image’s dimension legitimizes the word “Singular” in the name of the framework. Moreover, the dimension of \( L_f(x) \) should not depend on the choice of point \( x \) and must be minimal possible [23]. Accordingly, such a vector
field \( F(x, \varepsilon) \) can be decomposed into a “fast subfield” that belongs to the subspace \( L_f(x) \) and its complement that represents a “slow subfield”. If \( L_f(x) \) does not depend on \( x \), the vector field \( F(x, \varepsilon) \) would represent a linearly decomposed singularly perturbed vector field. Clearly, linearly decomposed singularly perturbed vector fields represent a non coordinate analogue of singularly perturbed systems of ordinary differential equations; moreover, this formal concept can be useful for practical applications only if it is supplied by an efficient identification algorithm of fast subfields.

In our previous works [14, 23] we have suggested a corresponding algorithm for linearly decomposed singularly perturbed vector fields. This algorithm is based on a global linear interpolation procedure for an original vector field that called a global quasi-linearization (GQL). This procedure is flexible enough and permits the adoption of an appropriate version of the global quasi-linearization for different applications. In the current work the scalar invariant version is discussed, and applied for model reduction of simple test examples, which, however, have all properties of a source term of typical reacting flow models.

2.1. Singularly perturbed vector fields: asymptotic definition

At the beginning, we remind you of a standard definition of vector bundles and then we use vector bundles as a formal substitute for non-linear coordinate systems. The use of vector bundles gives theoretical background for the non coordinate version of the SPS we are interested in. In the following the number of basic concept will be defined and outlined in brief.

**Definition 2.2** A real vector bundle \( \xi \) over a connected manifold \( N \subset R^m \) consists of a set \( E \subset R^m \) (the total set), a smooth map \( p : E \rightarrow N \) (the projection) which is onto, and each fiber \( F^k_x = p^{-1}(x) \) is a finite dimensional affine subspace. These objects are required to satisfy the following condition: for each \( x \in N \), there is a neighbourhood \( U \) of \( x \) in \( N \), an integer \( k \) and a diffeomorphism \( \varphi : p^{-1}(U) \rightarrow U \times R^k \) such that on each fiber \( \varphi \) is a homomorphism.

By this definition the dimension of fibers is constant.

**Definition 2.3** Call a domain \( V \subset R^n \) a structured domain (or a domain structured by a vector bundle) if there exists a vector bundle \( \xi \) and a diffeomorphism \( \psi : V \rightarrow W \) onto an open subset \( W \subset E \), where \( E \) is the total set of \( \xi \).

Now, we fix a parametric family of smooth vector fields \( \Phi(z, \delta) \) defined in a domain \( V \subset R^n \) for any \( 0 < \delta < \delta_0 \). Here \( \delta_0 \) is a fixed positive number and \( \delta \) is a small positive parameter. At the initial stage of the SPVF definition, the presence of the system’s small parameter is required.

A corresponding dynamical family of ODEs systems is

\[
\frac{dz}{dt} = \Phi(z, \delta).
\]  

**Definition 2.4** Suppose that \( V \) is a domain structured by a vector bundle \( \xi \) and a diffeomorphism \( \psi \). For any point \( z \in V \) call \( M_z := \psi^{-1}(p^{-1}(p(\psi(z))) \cap W) \) a fast manifold associated with the point \( z \). Call the set of all fast manifolds \( M_z \) a family of fast manifolds of \( V \).

By construction, any point \( z \in V \) belongs to only one fast manifold. If \( z \neq z_1 \) either \( M_z \cap M_{z_1} = \emptyset \) or \( M_z = M_{z_1} \). Additionally, the dimension of any manifold \( M_z \) should be the same. Denote this dimension by \( n_f \) and call it the fast dimension of \( \Phi \). Denote \( TM_z \) a tangent space to \( M_z \) at the point \( z \).

For a standard singularly perturbed system (see (5), (6)) \( M_z = R^{n_f} \) and \( \dim M_z = n_f \) correspondingly.

**Definition 2.5** A family of fast manifolds \( M_z \) is linear if there exists a fixed linear subspace \( L_f \) of \( R^n \) such that \( M_z = \{z\} + L_f \) for any \( z \in V \).
Call $L_f$ a fast subspace.

**Definition 2.6** A parametric family $\Phi(z, \delta) : V \rightarrow R^n$ of vector fields defined in a domain $V$ structured by a vector bundle $\xi$ and a diffeomorphism $\psi$ is an asymptotic singularly perturbed vector field if
\[ \lim_{\delta \rightarrow 0} \Phi(z, \delta) \subset TM_z \text{ for any } z \in V \text{ and the structure of domain } V \text{ is minimal for the vector field } \Phi(z, \delta) \text{ in the following sense. There is the proper vector subbundle } \xi_1 \text{ of the vector bundle } \xi \text{ such that } \Phi(z, \delta) \text{ is no an asymptotic singularly perturbed vector field in a domain } V \text{ structured by the sub bundle } \xi_1 \text{ and the same diffeomorphism } \psi. \]

This property of minimality means that it is not possible to reduce further the dimension of fast manifolds $\{M_z\}$ using subbundles. Hence, without loss of generality we suppose that a family of fast manifolds $\{M_z\}$ associated with a singularly perturbed vector field $\Phi(z, \delta)$ is always minimal. For a linear family of fast manifolds associated with a singularly perturbed vector field $\Phi(z, \delta)$ the property of minimality can be written in a rather simple way. If $L_f$ is a minimal fast linear subspace associated with a singularly perturbed vector field $\Phi(z, \delta)$, then dimension $n_f = \dim L_f$ can not be further reduced.

Call this minimal subspace $L_f$ a linear subspace of fast motions of $\Phi(z, \delta)$.

### 2.7. Decomposition of singularly perturbed vector fields

In this subsection we briefly outline a transition stage from SPVFs to formally decomposed vector fields. Accordingly, let us fix an asymptotic singularly perturbed vector field $\Phi(z, \delta)$.

**Definition 2.8** Call an asymptotic singularly perturbed vector field $\Phi(z, \delta)$ a uniformly asymptotic singularly perturbed vector field (or simply a uniform vector field) if
\[ \lim_{\delta \rightarrow 0} \sup_{z \in V} |Pr_z \Phi(z, \delta)| = 0. \]

Denote $\varepsilon := \sup_{z \in V} |Pr_z \Phi(z, \delta)|$ which is a new small parameter, which $\varepsilon < \varepsilon_0 = \sup_{z \in V} |Pr_z \Phi(z, \delta_0)|$. $F(z, \delta) := Pr_z \Phi(z, \delta)$ is the fast part of the original vector field and $G(z, \delta) := \frac{Pr_z \Phi(z, \delta)}{\sup_{z \in V} |Pr_z \Phi(z, \delta)|}$ is a slow part of $\Phi(z, \delta)$. Then, the vector field $\Phi(z, \delta)$ is formally represented as a linear combination of its fast and slow subfields i.e.
\[ \Phi(z, \delta) = F(z, \delta) + \varepsilon G(z, \delta). \quad (2) \]

The small parameter $\varepsilon(\delta)$ is a function of the small parameter $\delta$. Moreover if $\delta \rightarrow 0$, then $\varepsilon \rightarrow 0$. It can be seen that for any practical implementation of the proposed construction of singularly perturbed vector fields it is extremely important to find a way for evaluation of fast manifolds and/or to approximate the fast part of the vector field. For the moment we have this for the linear case i.e. for the case where all fast manifolds are parallel to a fixed linear subspace $L_f$.

### 2.9. Remarks on slow invariant manifolds

Before presenting results concerning fast manifolds, we make a few remarks about slow invariant manifolds. This is important as a complimentary part of the reduction procedure, meaning that the system can be reduced to either fast or slow manifolds correspondingly. Thus, let us suppose that $\Phi(z, \delta) = F(z, \delta) + \varepsilon G(z, \delta)$ is a singularly perturbed vector field. Hence, the equation
\[ F(z, \delta) = 0 \] represents a "fast isocline" of the vector field \( \Phi(z, \delta) \). If its solution defines a manifold

\[ S_0 = \{ z : F(z, \delta) = 0 \} \tag{3} \]

with tangent spaces transversal to fast manifolds (this manifold has the dimension \( n_s = n - n_f \)), then by using local charts of the corresponding vector bundle and a standard local representation of manifold \( S_0 \) as a graph of a vector function it is possible to prove existence of a slow invariant manifold \( S \) for which \( S_0 \) is a zero approximation (\( \delta = 0 \)) similar to that in the standard theory of singularly perturbed systems (see e.g. [19]).

Of course this restriction on \( S_0 \) does not hold for all points of \( S_0 \) in any realistic situation. Even if \( S_0 \) is a manifold it can happen that for some of its submanifold a tangent space is not transverse to fast manifolds. In this case the submanifold represents manifold of turning (jumping) points of \( S_0 \), where slow dynamics can be changed by fast one. In this paper we will avoid any discussion about these delicate submanifolds and will consider it in future work.

The dynamics on \( S_0 \) are the dynamics of the slow subfield \( G(z, \delta) \) which belongs to the tangent bundle of \( S_0 \). In order to obtain the next approximation of the slow invariant manifold let us differentiate the fast vector field \( F(z, \delta) \) and use the original vector field \( \Phi(z, \delta) = F(z, \delta) + \varepsilon G(z, \delta) \); thus we obtain an expression

\[ S_1 = \{ z : F_z(z, \delta) (F(z, \delta) + \varepsilon G(z, \delta)) = 0 \} \tag{4} \]

where terms of order \( o(\delta) \) are neglected. Repeating differentiation of approximations the highest orders can be easily obtained. This procedure, in some sense, coincides with evaluation of the implicit form of the invariant slow manifolds (see e.g. [19], [23]).

3. Fast Manifolds (Linear Case)

Theoretically everything above is simple, but in reality, for practical complex models, a small parameter \( \delta \) as well as a suitable decomposed form, are unknown, which restricts considerably the application of the proposed asymptotic theory. Moreover, it is very often the case that an "analytical" form of the system is not available as well. In applications, normally, it just comprises a number of subroutines that calculate of the thermochemical properties of chemically reacting species (the source term = chemical kinetics mechanism), their transport properties and hydrodynamic field, which then are coupled/incorporated through the first principles represented by the so-called reacting Navier-Stokes equations system.

In this section we outline an implementation of developed asymptotic theory in the simplest possible case of linear fast manifolds. Note, however, that for many engineering applications the assumption that \( L_f \) does not depends on \( z \) is found to be natural or can efficiently be used as an approximation to the actual family of fast manifolds. Moreover, restricting ourselves by homogeneous reactors, it means that the transport properties and their influence on the reduced model may be neglected, yielding the system of ODEs consisting of the source term only.

3.1. Fast-slow decomposition (SPS form)

In this subsection the connection between the SPVF and the SPS forms of the system is given explicitly. Similar to above, consider a uniformly asymptotic singularly perturbed vector field \( \Phi(z, \delta) \) and suppose that the fast subspace \( L_f \) does not depend on \( z \) and \( \dim L_f = n_f \). Then, the vector field \( \Phi(z, \delta) \) is a sum of two vector fields \( \Phi_f(z, \delta) := P_{r_f} \Phi(z, \delta) \) and \( \Phi_s(z, \delta) := \Phi(z, \delta) - P_{r_f} \Phi(z, \delta) \). Here \( P_{r_f} \Phi(z, \delta) \) is a projection of \( \Phi(z, \delta) \) onto the fast subspace \( L_f \), while \( \Phi_s(z, \delta) \) is a corresponding projection of \( \Phi(z, \delta) \) onto the linear slow subspace \( L_s \).

The uniformity condition permits us to represent a uniformly singular vector field and the corresponding dynamical system (1) as a standard singularly perturbed system (SPS).
corresponding construction is the following: first, suppose that \( x := Pr_f z \) and \( y := Pr_s z \) are fast and slow variables that represents a new coordinate system, with \( n_f \) fast variables \( x \) and \( n_s = n - n_f \) slow variables \( y \); \( \varepsilon := \sup_{z \in V} |Pr_s \Phi (z, \delta)| \) is a small parameter, \( \varepsilon < \varepsilon_0 = \sup_{z \in V} |Pr_s \Phi (z, \delta_0)| \); \( F (x, y, \delta) \) is a representation of \( F (z, \delta) := \frac{Pr_f \Phi (z, \delta)}{Pr_s \Phi (z, \delta)} \) in the new coordinate system \( (x, y) \) and \( G (x, y, \delta) \) is a representation of \( G (z, \delta) := \sup_{z \in V} Pr_f \Phi (z, \delta) \) in the new coordinate system \( (x, y) \).

Hence the system (1) has the standard SPS form

\[
\frac{dx}{d\tau} = F (x, y, \delta) \tag{5}
\]

\[
\frac{dy}{d\tau} = \varepsilon G (x, y, \delta) \tag{6}
\]

in the new coordinate system \( (x, y) \).

Note that the small parameter \( \varepsilon \) is a function of the small parameter \( \delta \), and if \( \delta \to 0 \), then \( \varepsilon \to 0 \).

3.2. Non-asymptotic decomposition

Obviously, the definition of an asymptotic singularly perturbed vector field \( \Phi (z, \delta) \) can not be useful unless \( F (z, \delta), G (z, \delta) \) and small parameters \( \delta, \varepsilon (\delta) \) are unknown. However the main geometrical idea is still useful if some previous knowledge about a scaling is available. It means that some “small” number \( \varepsilon_0 \) is fixed for corresponding processes (models) and any parameter \( \varepsilon < \varepsilon_0 \) can be considered as a small parameter. Thus, non asymptotic definition of a singularly perturbed vector field will depend on the scaling \( \varepsilon_0 \).

Now, suppose a smooth vector field \( \Phi (z) \) defined in a structured domain \( V \subset \mathbb{R}^n \),

\[
\frac{dz}{dt} = \Phi (z) \tag{7}
\]

and \( L_f \) is the fast subspace. Here \( \sup_{z \in V} |Pr_s \Phi (z)| < \varepsilon_0 \) and \( x := Pr_f z, y := Pr_s z \) are fast and slow variables that represent a new coordinate system with \( n_f \) fast variables \( x \) and \( n_s = n - n_f \) slow variables \( y \); \( \varepsilon := \sup_{z \in V} |Pr_s \Phi (z)| \) is now the small system parameter; \( F (x, y) \) is a representation of \( Pr_f \Phi (z) \) in the new coordinate system \( (x, y) \) and \( G (x, y) \) is a representation of \( \frac{Pr_f \Phi (z)}{\sup_{z \in V} |Pr_s \Phi (z)|} \) in the new coordinate system \( (x, y) \).

Hence the system (1) has a standard SPS form

\[
\frac{dx}{d\tau} = F (x, y) \tag{8}
\]

\[
\frac{dy}{d\tau} = \varepsilon G (x, y) \tag{9}
\]

in the new coordinate system \( (x, y) \).

On the one hand side this formal description is useless without an efficient procedure that will permit evaluating a fast subspace \( L_f \) for a singularly perturbed vector field \( \Phi (z) \), but on the other hand the knowledge about the fast subspace is only what we require for proper transformation of the original (7) to the SPS form (8, 9). In the following the so-called quasi-linearisation procedure of vector fields is presented as a basis of general construction and using the above notation.
3.3. Evaluation of fast subspaces

Suppose \( \Phi(z) \) is a uniform singularly perturbed vector field defined in a structured domain \( V \). Then \( \Phi(z) \) can be represented as a sum \( \Phi(z) := F(z) + \varepsilon G(z) \), where \( F(z) \) is a fast part of the vector field \( \Phi(z) \), \( \varepsilon G(z) \) is a slow part of the vector field \( \Phi(z) \), and \( \varepsilon \) is an unknown system small parameter.

The main theoretical questions that algorithm should answer (automatically) are the following

- Whether the given vector field can be decomposed (linearly) or not?
- What is the system small parameter?
- What is the minimal dimension of the decomposed form required for reduction purposes?
- How the fast subspace can be found?

In order to answer these questions let us follow the geometrical structure we have constructed. First, we assume that the system under consideration, (7), belongs to a family of uniformly singular perturbed vector fields with linear fast manifolds. This means that for an arbitrary point \( z \) in the defined domain \( V \) the vector field \( \Phi(z) \) is almost tangent to the fast subspace \( L_f \). The defect is due to a finite value of the small system parameter, which is obviously not zero for the particular realization. Note additionally that, we will not even try to find \( \delta \) because only the parameter \( \varepsilon = \varepsilon(\delta) \) is of practical importance. Hence, in order to find the fast subspace, we suggest that we fix arbitrary \( n \) points \( z_1, ..., z_n \in V \) and study they images under the vector field.

We call an \( n \times n \)-matrix \( T := [\Phi(z_1), ..., \Phi(z_n)] \) (as columns) a quasi-linearisation matrix of the vector field \( \Phi(z) \) associated with points \( z_1, ..., z_n \).

In the case in which all points \( Z = \{ z_1, ..., z_n \} \) are in general position (see discussion of the choice below) the linear structure of the matrix \( T \) should contain the information about the fast subspace. To illustrate this reconsider it in the asymptotic form as it has been previously described. Namely, if we have \( T(Z; \varepsilon) := [\Phi(z_1, \varepsilon), ..., \Phi(z_n, \varepsilon)] \) with explicit system small parameter, then due to the representation \( \Phi(z, \varepsilon) := F(z, \varepsilon) + \varepsilon G(z, \varepsilon) \) the matrix \( T \) splits into a sum

\[
T(Z; \varepsilon) = T_f(Z; \varepsilon) + \varepsilon \, T_s(Z; \varepsilon)
\]

of the so-called “fast” and “slow” matrices \( T_f \) and \( \varepsilon \, T_s \). In the limit \( \varepsilon \to 0 \), \( T(Z; 0) = T_f(Z; 0) = [F(z_1, 0), ..., F(z_n, 0)] \) and, consequently, linear column space of \( T \) will define the fast subspace \( L_f \). Now, for a finite, but small enough (asymptotically) value of \( \varepsilon \) and for suitable choice of \( Z \) the matrix \( T \) should have two groups of eigenvalues: \( n_f \) “large” eigenvalues \( \lambda^f_1, ..., \lambda^f_{n_f} \), (their eigenvectors asymptotically form a basis of the fast subspace \( L_f \)) and \( n_s \) “small” eigenvalues \( \lambda^s_1, ..., \lambda^s_{n_s} \) (that tend to zero when \( \varepsilon \) tends to zero). It allows decomposition of the matrix \( T \) by using invariant subspaces of eigenvectors that correspond to these two groups of eigenvalues:

\[
T = (Q_s \quad Q_f) \cdot \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \cdot \begin{pmatrix} \tilde{Q}_s \\ \tilde{Q}_f \end{pmatrix}, \quad (10)
\]

where \( \tilde{Q} = Q^{-1} = (Q_s \quad Q_f)^{-1} = (\tilde{Q}_s \quad \tilde{Q}_f) \), and \( N_s, N_f \) block matrices (or diagonal matrices \( N_s = \text{diag} \{ \lambda^s_1, ..., \lambda^s_{n_s} \}, N_f = \text{diag} \{ \lambda^f_1, ..., \lambda^f_{n_f} \} \) if all eigenvalues are different). Hence, corresponding dimensions, invariant subspaces and the system small parameter \( \varepsilon \) are defined/estimated on a basis of the so-called gap condition

\[
\varepsilon = \min \left( \frac{\lambda_i(T)}{\lambda_{i+1}(T)} \right), \quad n_s = i, \ n_f = n - n_s, \quad (11)
\]
for ordered eigenvalues \( i < j \iff |\lambda_i| \geq |\lambda_j| \) of \( T \). To define the gap one has to use *a priori* knowledge about smallness; namely, one should have the upper bound for the system small parameter \( \varepsilon_0 \) and, then, use this estimate in (11) as \( \varepsilon \leq \varepsilon_0 \).

3.4. Scalar invariant form and new criteria

Of course efficiency of the procedure above essentially depends on the choice of the so-called reference set \( z_1, \ldots, z_n \). It is obvious that this is a crucial point of the algorithm. Very general and practical recommendations for the choice that must be adopted for each particular model are the following

- the vector field \( \Phi (z) \) should present essentially “different” behavior for different points \( z_i \in Z \); it means the fast subspace should be completely described by the set \( Z \),
- points in the reference set must be “far” from the slow manifold (if it exists), because in the vicinity of the slow manifold there is no decomposition of motions,
- the vectors in \( Z \) have to be rather “far” from each other and should cover the domain “uniformly” representing the vector field in the whole domain of interest in the state space.

Another important problem with application is the invariance with respect to the normalization or, more generally, with respect to any linear transformation of the original system’s coordinates. It is clear that if one were to change the scale of one variable, this would influence the overall hierarchy. Namely, using the following simple change of variable for the state vector

\[
\tilde{z} = \text{diag}\{1, \ldots, \varepsilon, \ldots, 1\} z,
\]

we can obtain, in the new coordinates, the perturbed decomposition

\[
\frac{d\tilde{z}}{dt} = \text{diag}\{1, \ldots, \varepsilon, \ldots, 1\} \Phi \left( \text{diag}\{1, \ldots, \frac{1}{\varepsilon}, \ldots, 1\} \tilde{z} \right).
\]

As we see in this illustrative example, one more “slow” variable can artificially appear during the GQL analysis as defined above due to normalization (take, for instance, the vector field \( \Phi = (1, 1, \ldots, 1) \)). It means that the original version of global quasi-linearization procedure (GQL), as proposed in previous papers, can be safely applied only to “normalized” systems having the same range of orders of magnitude of all functions in the Right Hand Sides (RHSs). In applications, however, it is very often the case that systems are not dimensionless. Therefore such systems cannot be treated by the original version of the GQL approach without a proper non-dimensionality procedure adopted beforehand.

To overcome this problem and to make the algorithm applicable to the system in dimensional form as well, we suggest to use both \( \{z_1, \ldots, z_n\} \) and \( \{\Phi (z_1), \ldots, \Phi (z_n)\} \) as column matrices and define a new matrix \( \tilde{T} \) of a modified version of the global quasi-linearisation (GQL) as follows

\[
\tilde{T} := [\Phi (z_1), \ldots, \Phi (z_n)] [z_1, \ldots, z_n]^{-1}.
\] (12)

This matrix has a simple geometrical interpretation. It is the matrix of linear mapping that transforms points \( z_1, \ldots, z_n \) to \( \Phi (z_1), \ldots, \Phi (z_n) \). It is easy to check that this version is scalar invariant in the following sense: its eigenvalues do not change under any linear transformation of the original system’s coordinates.

To show this feature of the modified approach (12), first, take any non singular linear transformation \( A \) and change the coordinate system of (7) similar to before

\[
\tilde{z} = Az,
\]
yielding
\[
\frac{d\tilde{z}}{dt} = A \Phi (A^{-1}\tilde{z}) = \tilde{\Phi} (\tilde{z}) .
\]

Now we build the GQL for the new system
\[
\tilde{T} := \left[ \tilde{\Phi} (\tilde{z}_1), ..., \tilde{\Phi} (\tilde{z}_n) \right] [\tilde{z}_1, ..., \tilde{z}_n]^{-1} ,
\]
\[
\tilde{T} = A [\Phi (z_1), ..., \Phi (z_n)] \left( A [z_1, ..., z_n]^{-1} \right) \equiv AT A^{-1} .
\]

This last means that the new GQL has the same eigenvalues as the old one. Thus, the modified version can be safely applied to the system in the dimensional form. The next crucial point is connected to the choice of the reference set. To make a particular choice the following steps have been proposed in [16]

(i) By performing quasi-stochastic uniform distribution, an "initial set" \( S_N = \{ z_1, ..., z_N \} \) consisting of points \( N \gg n \) uniformly distributed in the domain \( V \) is formed. Then, we calculate the mean value of the vector field over the sequence \( S_N \) as
\[
\bar{\Phi} = \frac{1}{N} \sum_{i=1}^{N} \Phi (z_i) ,
\]
and take a subset of \( S_N \) as follows
\[
S_K = \{ z_i \in S_N : \| \Phi (z_i) \| \geq \| \bar{\Phi} \| i = 1, .., K \} ,
\]
where \( i = 1, ..., K \), \( K = k \cdot n \), \( k \gg n \). The set \( S_K \) is called a "separated set" and consist of points which are “far” from the slow manifold in the following sense. The vector field at these points has values above average level and, therefore, can safely be used to evaluate the fast subspace. Note that any subset of length \( n \) of the control set \( S_K \) can be used as the reference set to obtain \( T \), but there is a degeneration problem of the chosen subset of the separated set if some of points will be close to one another. This can lead to degeneration of the matrix \([z_1, ..., z_n]\) and, consequently, to incorrect decomposition [16]. Accordingly, not every subset of \( S_K \) of length of \( n \) can be safely applied as the reference one.

(ii) To solve the problem with degeneration we have to take a subset of vectors that spans the simplex of volume which is compared to the volume of the domain \( V \). Therefore, we build up the sequence of GQL approximations \( T_i \), \( i = 1, ..., k \) based on subsets of the control set
\[
Z_i = \{ z_{i-1+1}, ..., z_{i+n} \} ;
\]
and select only those subsets \((14)\), which have \( |\det ([Z_i])| \) above the average level over all subsets: \( \bar{D} = \frac{1}{k} \sum_{i=1}^{k} |\det ([Z_i])| \). Denote by
\[
S_C := \{ Z_i : z_{ik} \in S_N : |\det ([Z_i])| \geq \bar{D} i = 1, ..., k \} ,
\]
the “control set” of ordered subsets of length \( n \) from set \( S_K \).
Now, in order to define the final GQL from the control set $S_C$ and to choose the best one it has been suggested in [16] to take the GQL that has the best decomposition (small parameter) for given dimension of the reduced model $n_s$. Hence, the final reference sequence $Z_{i^*} = \{ z_{(i^*-1)n+1}, \ldots, z_{i^*n} \}$ and the final GQL approximation are found simultaneously as

$$ T = T_{i^*} = [\Phi(z_{(i^*-1)n+1}), \ldots, \Phi(z_{i^*n})] [Z_{i^*}]^{-1} $$

by a maximal gap:

$$ i^* : \varepsilon = \min_i \left( \frac{|\lambda_{n_s}(T_i)|}{|\lambda_{n_s+1}(T_i)|} \right), \quad (16) $$

where $\lambda_j(T_i), j = 1, \ldots, n$ are eigenvalues of $T_i$ ordered in increasing order by absolute values (see (11) above).

In this realization of the GQL it has been assumed that one knows (possibly by additional analysis) the desired dimension of the decomposition. In this case it has been shown [16] that the final choice of the reference set works quite well, but unfortunately, for the dimension analysis and for hierarchy investigation the suggested final choice of the reference set is not sufficient.

The lack of the general criteria for the final sorting and choice of the reference set restricts considerably the application range of the GQL approach. For these reasons, in the current study, we overcome this drawback and suggest an alternative procedure for the final choice of the reference set based on geometric type invariants.

### 3.5. Accurate choice of the control set

To make the method self-consistent and independent of additional dimension analysis, we require from the final GQL that it should reproduce by linearized version some geometrical invariants of the original vector field.

For this, we define the following invariants of the vector field based on an integral of the characteristic polynomial coefficients of the differential $J_\Phi(z)$ of the vector field $\Phi(z)$:

$$ I_j(\Phi; V) = \int_V a_j(z; \Phi) \, dz, \quad j = 1, \ldots, n \quad (17) $$

where

$$ f_{J_\Phi(z)}(t) = t^n + a_1(z; \Phi) t^{n-1} + \ldots + a_n(z; \Phi), \quad J_\Phi(z) = \Phi_z(z), \quad (18) $$

The same invariants for the vector field, produced by the GQL procedure, are the following:

$$ I_j(T; V) = a_j(T) \, |V|, \quad j = 1, \ldots, n. \quad (19) $$

There is a clear interpretation of the integral of the last invariant giving the volume of the image of the domain of interest $V$: $|\text{Im}(\Phi(V))| \equiv |I_n(\Phi; V)|$.

Other integrals do not have such clear geometrical interpretations, but certainly have connection to the geometrical structure of the vector field. Hence, the final choice of the GQL is performed on a basis of the following functional

$$ \Pi(T; V) = \sum_{I_j(\Phi; V) \neq 0} \left| \frac{I_j(T; V) - I_j(\Phi; V)}{I_j(\Phi; V)} \right|. \quad (19) $$

The chosen GQL minimizes the functional above over the control sequence.
Figure 1. System dynamics (21) in the $(x, y)$ plane. The vector field is shown by arrows, GQL fast subspace is given by the red line, blue line is corresponding slow curve, solid black lines are system trajectories for arbitrary initial points.

\[ T^* : \min_{i=1,\ldots,k} (\Pi (T_i; V)) = \Pi (T^*; V). \]  

(20)

The rest is standard, the spectrum of $T^*$ answers the question about existing hierarchy, a gap condition can be used for definition of the decomposition dimension and small system parameter, invariant subspaces of two groups of eigenvalues defines the fast and slow subspaces etc.

4. Examples and Discussion

In this section a number of examples are given which are intended to illustrate and verify the method above.

4.1. 2D simple example

In the first example, we take an artificial 2D ODE system and apply our method to see what is possible to obtain for the system without the system small parameter and/or without a clear decomposition of motions.

\[ \begin{aligned}
\frac{dx}{dt} &= -3x^3 + y^2 \\
\frac{dy}{dt} &= x^2 - xy
\end{aligned} \]  

(21)

The results for $V = [0, 1] \times [0, 1.2]$ are shown in Fig. 1, where the red line is an approximation of the fast motion and blue line represents the slow curve. The result of the GQL analysis for $N = 2000$ is summarized below

\[ T = \begin{pmatrix} -2.67 & 0.58 \\ 0.93 & -0.93 \end{pmatrix}, \quad Q = \begin{pmatrix} -0.690 & -0.27 \\ 0.4 & -0.96 \end{pmatrix}, \]

\[ \lambda (T) = \{-2.94, -0.66\}. \]
4.2. 2D SPS with hidden hierarchy

The second example has been used in our previous work [23]. Here we use it again for illustration of the problem with scales. Consider the system in the standard SPS form:

\[ \varepsilon \frac{dx}{dt} = -(x + \sin(x) + \sin(y)) \]
\[ \frac{dy}{dt} = -y \]  

then we rotate the system coordinates according to

\[ \begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} x \\ y \end{pmatrix}, \quad A = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \]  

and rescale the variables by

\[ \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1/\varepsilon & 0 \\ 0 & 1 \end{pmatrix} A \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 7.07 & -7.07 \\ 0.70 & 0.70 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \]  

Now, apply the suggested global quasi-linear approximation (GQL) in order to redefine the existing decomposition in the \((x, y)\) phase plane for these new two systems (23)-(24).

The decomposed structure of the three resulting systems is presented and summarized in Fig. 2. Below, the results of the GQL analysis are presented for the more interesting case (24)

\[ T = \begin{pmatrix} -7.11 & -28.95 \\ -0.61 & -3.89 \end{pmatrix}, \quad Q = \begin{pmatrix} -0.99 & 0.97 \\ -0.09 & -0.20 \end{pmatrix}. \]

\[ \lambda(T) = \{-10.01, -1.00\}. \]

4.3. Semenov’s thermal explosion model

The third example is the Semenov’s thermal explosion model, which illustrates the capability of the method to improve the fast manifolds even for the system in the standard SPS form [14, 19].

\[ \gamma \frac{dx}{dt} = y \exp\left(\frac{x}{1+\beta x}\right) - \alpha x \]
\[ \frac{dy}{dt} = -y \exp\left(\frac{x}{1+\beta x}\right) \]  

Figure 2. Left figure shows the system dynamics (22) in the \((x, y)\) state plane of original variables with \(\varepsilon = 0.1\); center figure - shows \((u, v)\) plane \((\theta = -\frac{\pi}{4})\) without rescaling (23), and the right figure represents \((u, v)\) plane according to (24). The magenta curve represents the slow manifold according to the standard SPS (RHS of the first equation (22)) in the original and new coordinates.
Figure 3. Left figure slows the system dynamics (25) in the \((x, y)\) plane with adiabatic (magenta) and GQL (red) directions of the fast motions, solid lines are system trajectories, blue line is an approximation of the system slow manifold (3); right figure - the same as in left, but with blue curves representing the next order of approximation of the slow manifold (4), where dashed line is the slow manifold of the standard SPS theory. The system parameters are \(\alpha = 2.2, \beta = 0.025, \gamma = 0.05\).

The results for \(V = [0, 6] \times [0, 1.2]\) are shown in Fig. 3, where the red line is an approximation of the fast motion and blue lines represent approximations of the slow invariant curve. As above, the result of the GQL analysis for \(N = 2000\) is given below

\[
T = \begin{pmatrix} 282.48 & 656.90 \\ -16.32 & -32.84 \end{pmatrix}, \quad Q = \begin{pmatrix} 0.99 & -0.92 \\ -0.05 & 0.38 \end{pmatrix},
\]

\[
\lambda (T) = \{243.71, 5.92\}.
\]

This example clearly shows that even for the standard SPS system the method is capable of improving the fast direction, which certainly deviates from \(y = Const\) for asymptotically small but finite system small parameter.

4.4. 3D Michaelis-Menten enzyme model

The final example is the 3D Michaelis-Menten model [24–26]. It is considered here in order to verify the suggested method and rediscover a hierarchical structure of this model. A simplified mathematical model consists of three ordinary differential equations

\[
\begin{align*}
\frac{dx}{dt} &= -xz + L_1 (1 - z - \mu (1 - y)) \\
\frac{dy}{dt} &= -L_3 y z + \frac{L_4}{L_2} (1 - y) \\
\frac{dz}{dt} &= \frac{1}{L_2} \left( (-x z + 1 - z - \mu (1 - y)) + \mu \left( -L_3 y z + \frac{L_4}{L_2} (1 - y) \right) \right)
\end{align*}
\]

The system parameters equal to \(L_1 = 0.99, L_2 = 1, L_3 = 0.05, L_4 = 0.1, \mu = 1\) and \(V = [0, 2] \times [0, 2] \times [0, 1.5]\); \(P_m = (1, 0.5, 1)\).

The system (26) has two (1D and 2D) subsequent slow manifolds (see [14] for detail) due to three sufficiently different time scales present in the system. Figure 4 shows typical trajectories of system solutions, where the red arrow corresponds to the fast manifold direction of the GQL method at the arbitrary chosen initial point \(P_m\).
In this example, with the help of the fast subspace (direction) the slow surface equation can be obtained analytically

\[ S_0 = \{ (x, y, z) : z = \frac{-0.05 (1 - y) - 1.41 y}{-1.41 (1 + x) - 0.02 y} \}, \]

for the following eigenvalues of \( T \)

\[ \lambda (T) = \{-2.76, -0.16, -0.003\}. \]

The discovered hierarchy, based on the eigenvalues above, clearly shows the existence of three different time scales (we see two gaps between eigenvalues at least of one order of magnitude), which exactly corresponds to the overall dynamical structure in Fig. 4.

5. Conclusions

In this work the theoretical framework of Singular Perturbed Vector Fields (SPVF) is further applied to reduce the problem. The main issue in this study is construction of an approximation for the actual (hidden) decomposition of the system dynamics into the so-called “slow” and “fast” motions. A robust, efficient, automatic and scalar invariant algorithm, which is based on the global quasi-linearization procedure (GQL) proposed in our previous papers, has been developed for kinetic models in dimensional form.

Using a number of test examples it has been shown that this approach can be successfully applied numerically for the construction of linear transformations of the original models to the standard SPS form. This makes applications of the powerful theory of singular perturbations possible.

These examples demonstrate also that the proposed method allows us to overcome the main difficulties which arise in numerical applications of the GQL (with reduced dimension analysis, small system parameter evaluation, fast subspace approximation, stability analysis etc.). Furthermore, it demonstrates that the suggested method, as well as its theoretical framework,
has a potential for construction of efficient numerical schemes for the automatic identification of the system multi-scale hierarchy with subsequent use of the corresponding decomposition for model reduction purposes.

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