Novel Numerical Decomposition Approaches for Multiscale Combustion and Kinetic Models

V Bykov\textsuperscript{1}, I Goldfarb\textsuperscript{2} and V Gol'dshtein\textsuperscript{2}

\textsuperscript{1} Institute of Technical Thermodynamics, Karlsruhe University (TH), Kaiserstrasse 12, Karlsruhe 76131, Germany
\textsuperscript{2} Department of Mathematics, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva 84105, Israel
E-mail: goldfarb@cs.bgu.ac.il

Abstract. A general theoretical procedure of decomposition of original multiscale system of ODEs into fast and slow subsystems is presented. Multiscale systems arise in modelling of chemical, biochemical, mechanical systems. The performed analysis shows that existing algorithms can be interpreted as possible realizations of the general framework for identification of slow invariant manifolds (slow motions). The aim of this framework is a decomposition of the original system of equations into two separate sets - fast and slow sub-systems. The analysis is based on a new concept of a singularly perturbed vector field. General procedures for decomposition of singularly perturbed fields onto fast and slow parts are presented and this permits us to develop the quasi-linearization method for identification of the fast and the slow subprocesses for complicated kinetics and combustion problems. Application of the suggested numerical technique (the quasi-linearization method) demonstrates that a number of the uncovered restrictions on existing numerical procedures are successfully overcome. The proposed numerical procedure is applied to the highly non-linear problems of mathematical theory of combustion and demonstrates an essentially better performance with respect to existing ones.

1. Introduction

Mathematical models of chemical, biochemical and mechanical systems are often formulated as a large set of differential equations which, for the purpose of numerical and/or analytical analysis, it is often desirable to reduce to a smaller system with a comparatively small loss of accuracy. Experience shows that a large set of differential equations describing complex chemical or mechanical phenomenon generally has a number of different time scales of sub-processes. This hierarchical structure allows one to apply various asymptotic approaches for analysis of the system dynamics. In a geometrical interpretation of phenomenon dynamics, one can describe the multi-scale hierarchy as a progressive motion through surfaces of lower and lower dimensionality (these surfaces are called invariant manifolds). At present there are a number of asymptotic tools able to treat the multi-scale system of equations. An incomplete list includes the computational singular perturbation CSP method [24, 25, 28, 31], the method of integral manifolds (MIM) [7, 38, 18, 2], an approach based on intrinsic low-dimensional manifolds (ILDM) [27, 26]. Most of these numeric tools were developed to uncover a slow stable manifolds. The present paper considers an arbitrary trajectory from another standpoint and focuses on both the slow and the fast stages of the real system dynamics. The aim of the research is to elucidate the importance of
these two distinct types of the system behaviour (fast and slow) and to develop a new combined approach to decomposition technique, which will contain the best features of the currently used techniques and will be free their disadvantages. The present study represents the first work of the series of papers, which will be devoted to research in this direction.

Let us give a bit more detailed explanation. Many physical, biological, chemical and mechanical systems are characterized by a large number of unknowns and a wide range of temporal or spatial scales. These scales govern the underlying differential equations and create serious difficulties (stiffness) for solution evolution, no matter which approach - analytical or numeric - is chosen. In order to address the issues of both stiffness and physical understanding, a variety of asymptotic tools were developed, which explore the existing gap in scales. Many of the existing methods, which were developed for the decomposition of the original system of ODEs, were primarily proposed for the investigation of combustion phenomena. Normally, an arbitrary mathematical model for gas-phase or multiphase chemical reaction systems consists of a large set of partial differential equations, which describe the time-dependent development of all the properties that determine the state of the system. The governing processes (i.e., flow, molecular transport, chemical reactions) occur at time scales that differ by orders of magnitude. The presence of the different time scales allows us to introduce in a very natural way small parameters characterizing the gap between various levels of the hierarchy. After suitable non-dimensionalization the dimensionless system obtained contains corresponding small parameter(s) involved both in right and left sides of the considered system of ODEs.

Note that decomposition of complex systems into simpler subsystems is de facto almost universally used in engineering and physics applications. It allows the numerical simulation to focus on low dimensional subsystems, thus avoiding substantial difficulties and instabilities related to numerical simulation of the original systems. Special rules are normally introduced to incorporate the results of numerical simulation of the subsystems into the general scheme of the simulation of the whole system.

Nevertheless, existing approaches to the decomposition of the original system of ODEs have a number of common properties, which represent some kind of "philosophy" of this method. The basic principles of this philosophy may be formulated as follows: (1) there is the single globally stable (attractive) manifold in the phase space; (2) there is the single singular point (of the system under consideration), which belongs to the stable manifold. Under these assumptions the fast period of the motion is of minor importance due to the following reasons: a time of the fast motion is of no importance and the point of intersection between the fast part of the trajectory and the slow manifold is of no importance. According to this philosophy, the main part of the dynamics, which is of real interest for a researcher or an engineer, belongs to the stable manifold. As a result of these basic principles, the main goal of the numerical algorithm developed (ILD M, SPC, inertial manifolds, etc) is the localization of this single stable slow manifold.

The systems of ODEs, which are of real industrial interest, do not met the basic principles of the aforementioned philosophy. Firstly, it would be worthwhile to note here, that the initial point (that corresponds to initial data) is normally located far from the stable slow manifold (the manifold has much lower dimension than the phase space does, therefore, the probability of the situation, when the initial point belongs to a small neibourhood of the real slow manifold is close to zero). Secondly, even simple analytical models demonstrate the fact that a slow manifold is not necessary unique and distinct branches of this manifold can demonstrate different types of stability. Thirdly, the relative location of the initial point and the real slow manifold and direction of the fast motion (normally its is the first stage of the system trajectory) are crucial for the evaluation of the intersection point and, in turn, for the choice of a branch of the slow manifold. Distinct branches of the slow manifold can demonstrate very different dynamics, therefore a global behaviour of the considered system depends crucially on the initial point’s
location. This fact is well known for thermal explosion models (for example, this allows us to
distinguish explosive and non-explosive regimes, for example).

In light of the arguments mentioned above and thanks to the extended experience of the
authors in the field of qualitative investigation of the dynamics of various system of ODEs,
dealing with combustion problems, the authors decided to concentrate both on the fast and
slow parts of an arbitrary trajectory and transient zones between distinct branches of the stable
manifold.

An outline of the paper is as follows. Section 2 contains our general thoughts concerning
the possible decomposition of an arbitrary system of ODEs into slow and fast sub-systems.
The Section starts with basic information useful for the rest of the article, namely, a general
description of the so-called singularly perturbed system (SPS) of ordinary differential equations
(ODEs). Following a description of the basic properties of the SPS of ODEs, we discuss
peculiarities of the asymptotic analysis of an arbitrary system of ODEs with small but finite
parameter and a possible multiple scales character of an arbitrary system (internal hierarchy),
which is generally “hidden” within the system. Section 3 is devoted to the short description of the
method of integral (invariant) manifolds, which serves as the reference point in verification of
the proposed numerical algorithms. Section 4 represents the authors’ general view on the geometrical
interpretation of the fast and slow motions of the system under consideration. Special attention
is drawn to the case of practical interest (so called singularly perturbed vector fields), when
the hierarchy of the system is “hidden” and can not be easily verified. Section 5 discuss
various approaches to system decomposition. It is shown that there is a general framework
of local/global approaches, which can be realized in an infinite number of ways. This general
framework for the evaluation of the fast and slow variables by a corresponding transformation of
coordinates is formulated for an arbitrary system of ODEs with “hidden” hierarchy. Following
the description of the general framework, a number handicaps of of the existing ILDM technique
are analyzed and a modification of the existing version of ILDM is suggested. It is shown,
that the proposed modification (TILDM) successfully overcomes some problematic points of the
ILDM machinery. In addition to a number of linear examples demonstrating the nature of the
problems, a mathematical model of the ignition of a cold fuel spray in a hot combustible mixture
is studied using the suggested modification. Following the subsections devoted to an analysis
of the location of the slow manifolds, a method for an approximation of the fast manifolds
is presented and its application to the realistic problem of numerical modelling of diesel fuel
combustion is demonstrated. Section 6 is devoted to a novel approach, which should allow one
to determine a transformation of the original coordinates, which is applicable within the domain
of interest (global quasi-linearization). Section 7 summarizes the main results presented in the
manuscript.

2. Singly Perturbed Systems - General Comments
In the present section we will present the authors’ thoughts concerning the possible
decomposition of a system’s dynamics into the fast and slow stages.

2.1. Singular perturbed systems
Singly perturbed systems (SPSs) are systems containing ordinary differential equations,
which exhibit dynamic behaviour evolving two (or more) vastly different time scales [2, 21, 7,
38, 18]. The conventional form of a singly perturbed system consists of a set of equations in
which derivatives of a number of variables are multiplied by a small parameter(s)

$$\varepsilon \frac{dX}{dt} = F(X, Y, \varepsilon)$$

(1)
In the general case, the RHS of the equations of the system (1)-(2) can depend on the small parameter $\varepsilon$. It is worthwhile to mention here, that the presentation of the original system in the form of the set (1)-(2) is to some extent a simplification. The general problem is normally harder than that described by the system (1)-(2) due to the possible presence of a large number of different timescales (the set (1)-(2) describes the pair of them only) and an absence of the explicit small parameter(s). However, the simplification made above does not effect the nature of the analysis performed. When the parameter $\varepsilon$ tends to zero, or the parameter $\varepsilon$ is small with respect to unity and the functions in the RHS of the equations (1)-(2) are of the same order (at least, in some bounded domain), the system (1)-(2) exhibits a dynamical behaviour characterized by a presence of two sufficiently different time scales. The difference between the rate of changes of the two vectors $(F, G)$ is determined by the small parameter $\varepsilon$. For our further convenience in the present paper we will suppose that both functions in the RHS of the equations (1)-(2) are sufficiently smooth (infinitely differentiable). Additionally, we assume that the RHS of the equations do not contain the time-like variable $t$ in an explicit form (we will restrict ourselves to autonomous systems only). Note here that a rate of change of the vector $X$ tends to infinity when $\varepsilon \rightarrow 0$ (assume that $F(X,Y,\varepsilon) \neq 0$). According to this elementary analysis of the Eqs. (1)-(2) the first of the two equations is called the fast sub-system, whilst the second is called the slow sub-system.

2.2. Asymptotic analysis - peculiarities with a finite value of the small parameter

Note, that there is a principal difference between theoretical asymptotic analysis under the assumption that $\varepsilon$ tends to zero and the analysis of the realistic case, when the small parameter $\varepsilon$ is small but finite. This fact essentially affect our possibility to apply the conventional machinery of asymptotic theory to this system. Under this presumption (finite value of $\varepsilon$), the aforementioned subdivision is correct under a number of additional restrictions allowing us to consider the system (1)-(2) as SPS. In particular, the functions $F(X,Y,\varepsilon)$ and $G(X,Y,\varepsilon)$ should be of the same order. Additionally, the system (1)-(2) can be considered as SPS within the bounded domain. The last restriction can be easily understood, because if the characteristic size of the domain is more then $1/\varepsilon$, a deviation of the trajectory from its fast direction can be large.

This situation was realized by a number of teams. The main philosophy of the the aforementioned approaches have a number of common properties, which represent some kind of "philosophy" of these methods. The basic principles of this philosophy may be formulated as follows: 1. There is the single globally stable (attractive) manifold in the phase space; 2. There is the single singular point (of the system under consideration), which belongs to the stable manifold. Under these assumptions the fast period of the motion is of minor importance due to the following reasons: the time of the fast motion is not importance, the point of intersection between the fast part of the trajectory and the slow manifold is also of no importance. According to this philosophy, the main part of the dynamics, which is of real interest for a researcher or an engineer, belong on the stable manifold. As a result of applying these basic principles, the main goal of the developed numerical algorithm (ILDM, SPC, inertial manifolds, etc) is localization of this single manifold.

2.3. Decomposition of the original system

In the context of our present study it would be reasonable to ask two main questions. The first one is related to our ability/inability to discover the presence of the internal hierarchy in the given system of ODEs and can for example be formulated in the following manner: can one determine whether a given system represents a system with "hidden" hierarchy? In more formal
language, can the given system be treated as a SPS, at least locally? Remind yourself that despite the fact that multi-scale systems are well known phenomenon in a number of human fields of scientific interests, no one may guarantee that the given system has a distinct scale "hidden" in its formulation. Once we have a positive answer to the previous question, the second question arises: is it possible to find a "global" (maybe "nonlinear") transformation of the original coordinate axes so that the original system of ODEs could be written in the conventional form of SPS? Both of the aforementioned questions sound rather reasonable and cumbersome. Nevertheless, the second, concerning a possible non-linear transformation looks much more complex than the first. Anyone who has a minimal experience in geometry knows how complicated it is to construct a "global" coordinate system with prescribed properties. The first question can be reformulated more formally. How can one found a direction of "fast" motion for a general system (1)-(2) for a fixed point \((X,Y)\) of the phase space? The trivial answer that the direction of fast motion is a direction of the vector field \((F(X,Y),G(x,y))\) is not helpful. We cannot extract from this answer any information about "slow" motion and invariant manifolds, except the trivial information, that any trajectory of the system is a one-dimensional invariant manifold. Such a trivial answer is not correct for any "global" singularly perturbed system, except for a linear one. This remark demonstrates the dual nature of any "local" concept. A "local" representation of the original system as a singularly perturbed one must be so global that "fast" motions must be more simple than original vector field. Any "global" singularly perturbed system of the type (1)-(2) demonstrates both properties. The fast motion is horizontal (simplest possible) and global (the whole phase plane). Let us formalize previous remarks for the multidimensional situation.

3. Method of Integral Manifolds - short summary

Theory of integral manifolds was developed for nonlinear mechanics [29, 38, 7]. This approach was adopted to problems of chemical kinetics and combustion in the book by Gol'dshtein and Sobolev [17], whose short English survey was published later ([18]. Later this approach was successfully developed and applied to various combustion problems - study of thermal explosion [1] in sprays [19, 14, 15, 30, 36, 35, 13], investigation of pressure-driven flame propagation in porous media [10, 5], research on thermal runaway in insulation material [11, 12]. Here we will formulate the main results relevant for applications of the geometrical version of the method of integral manifolds (MIM) to the considered problem.

Consider a singularly perturbed system (1)-(2) of ordinary differential equations, where \(X \in \mathbb{R}^m, Y \in \mathbb{R}^n, \varepsilon < < 1\) is a small positive parameter, functions \(F : U \times V \rightarrow \mathbb{R}^m, G : U \times V \rightarrow \mathbb{R}^n\) defined in the direct product of domains \(U \subset \mathbb{R}^m, V \subset \mathbb{R}^n\). Suppose that functions \(F, G, h_0\) have continuous derivatives of any order.

Set \(\varepsilon = 0\). We obtain an algebraic-differential system

\[
0 = F(X, Y) \quad (3)
\]

\[
\frac{dY}{dt} = G(X, Y) \quad (4)
\]

Suppose that equation (3) has solution \(Y = h_0(X)\) and this solution is isolated, i.e. there exists such a number \(\rho > 0\) that in the neighborhood \(\Omega := \{X|Y - h_0(X)| < \rho\) no other solution of the equation (3) exists. Suppose also that functions \(F, G, h_0\) are uniformly continuous together with their derivatives up to order \(k + 2, k \geq 1\).

A manifold (surface) \(M := \{(X, Y) : y = h(X, \varepsilon)\}\) is called an integral manifold of the system (1)-(2) if any phase trajectory \(\gamma(X, Y)\) of the system (1)-(2) that intersects \(M\) belongs to \(M\) in domain of existence of \(M\).

Let all eigenvalues \(\lambda_i(X), i = 1, 2, \ldots, n\) of the matrix \(B(x, t) = \frac{\partial G}{\partial y}(X, h_0(x))\) satisfy to the inequality \(Re(\lambda_i(x)) \leq -\alpha, \alpha > 0\). The general theory of integral manifolds states that
there is some \( \varepsilon_0 > 0 \) that for any \( \varepsilon < \varepsilon_0 \) the original system has a unique integral manifold \( M := \{(x, y) : y = h(x, \varepsilon)\} \) of the class \( C^k \) belonging to an \( \varepsilon \)-neighborhood of the slow (quasistationary) manifold \( M_0 := \{(x, y) : y = h_0(x)\} \), where \( y = h_0(x) \) is an isolated solution of the (2) with \( \varepsilon = 0 \).

Moreover there exist a unique representation \( h(X, \varepsilon) = h_0(X) + \sum_{i=1}^{\infty} \varepsilon^i h_i(X) \). For \( \varepsilon < \varepsilon_0 \) the series converges to the function \( h(X, \varepsilon) \). There is an effective analytical algorithm for evaluation of coefficients \( h_i(X) \) for arbitrary \( i \) (by iteration). It means that the slow manifold \( M_0 \) is an \( O(\varepsilon) \) approximation of the integral manifold \( M \), except at points where the assumption on its eigenvalues do not hold (so-called turning points).

The asymptotic series that represent integral manifold are not time-dependent and standard methods for the time-dependent asymptotic series are not relevant. Asymptotic series of integral manifolds are asymptotic expansion of "fast" phase variables \( Y \) with help of "slow" \( X \) phase variables.

The general theory produces a number of important conclusions. In particular, the fact, that the slow surface (slow manifold) \( M_0 \) is an \( O(\varepsilon) \) approximation of the integral manifold, permits us to write the slow Equation (37) on the slow surface \( M_0 \) (which has a lower dimension than the original system (1)-(2)) and to study the system dynamics on it.

The outcomes of the general theory cited above may be interpreted in the following practical way. Each solution of the system of Equations (1)-(2) can be presented as a trajectory in the phase space of the variables \( X \) and \( Y \). This trajectory can be subdivided into fast and slow parts. In the fast part, the slow variable \( Y \) is assumed to be constant (quasistationary). In the slow parts, the fast variable \( X \) changes with approximately the same rate as the slow one does (on the corresponding slow integral manifold fast and slow processes are balanced). The slow parts of the trajectory are located on the integral manifold \( M \) (a curve in the two-dimensional case). For purposes of qualitative analysis its zero approximation \( M_0 \) can be taken. This means that the application of the technique presented above to the solution of Equations (1)-(2) should start with the estimate of the relative rates of change of the variables and make a decision regarding which of them are fast and slow.

Further, suppose we deal with the more complicated case with several characteristic rates of change. Consider an arbitrary hierarchical level of the system. For processes of the same order, all the slower processes are assumed to be ‘frozen’, while all the faster processes are expected to reach their quasi-stationary state. Eventually, however, the processes under consideration at the corresponding hierarchical level approach their quasi-stationary state. It should be emphasized that this state of relative balance is temporary in the general case and these processes can become fast once again. This phenomenon seems not to be well understood and it is commonly believed that the processes always become quasistationary after the first quasi-relaxation. This was the main driving force behind the development of a more rigorous mathematical technique (partially cited above), namely, the geometrical asymptotic version of invariant manifolds \( M \). This theory represents a solid mathematical background for the analysis of the aforementioned systems.

4. Geometrical Interpretation

In this Section we will present the authors’ view on the issue of interpretation of the possible regimes of the system dynamics: considered earlier fast and slow motions.

4.1. Geometrical Interpretation of the Fast and Slow Motion

Consider system (1)-(2) in the two-dimensional case and divide the second equation of the system by \( \varepsilon \). The RHS of the re-written system represents the vector field \( (F(x, y), G(x, y)/\varepsilon) \) (note, that we use \( x \) instead of \( X \) and \( y \) instead of \( Y \) due to specific dimension of the system). To analyze the dynamics of the system in the \( (x, y) \) phase plane, it would be wise to divide the functions
\( \mathbf{F}(x, y) \) and \( \mathbf{G}_1(x, y) \) \( (\mathbf{G}_1(x, y) = \mathbf{G}(x, y)/\varepsilon) \). The fraction represents a derivative \( dy/dx \) or an inverse. Exclude from consideration neighbourhoods of the isoclines of the components of the vector field \( \mathbf{F}(x, y) = 0, \mathbf{G}(x, y) = 0 \). In the rest of the region, where the aforementioned conditions are valid, the absolute value of the derivative \( dx/dy \propto \varepsilon \) and the real trajectory almost coincides with the straight line parallel to the corresponding axes determined by the initial value of the appropriate variable \( (x = x_0 = const) \). Denote the ratio \( \mathbf{F}(x, y)/\mathbf{G}(x, y) \) by \( \zeta(x, y) \), which is obviously a function of the coordinates \( x, y \). The function \( \zeta(x, y) \) can be interpreted as a \textit{local} small parameter depending on the chosen point \( (x, y) \). Comparing the values of the function \( \zeta(x, y) \) in the different points of the region of interest, one can easily conclude that \( \sup \zeta(x, y) \propto (O(\varepsilon)) \).

Suppose now that we have not an \textit{a-priori} information concerning a presence of the internal (hidden) hierarchy in the system of the type

\[
\frac{dx}{dt} = \mathbf{F}(x, y) \tag{5}
\]

\[
\frac{dy}{dt} = \mathbf{G}_1(x, y), \tag{6}
\]

To uncover this property we are able to compare the values of the function \( \zeta(x, y) \). Once we found that there is a domain \( U \), where \( \sup \zeta(x, y) \) is much smaller than unity, we have a \textit{global} (valid within the aforementioned domain) small parameter which can be used for a subdivision of the fast and slow motions. Within the framework of the accepted notations, the fast motion in this case can be approximated by the constant (initial) values of the variable \( x \) \( (x = x_0 = const) \). The fast part of the real trajectory distincts from its approximation (fast motion according to our subdivision) by the order \( O(\varepsilon) \).

Note here that the situation, when one can come to a conclusion that the variables \( x \) and \( y \) are the slow and fast correspondingly within the bounded domain only, which size depends on the small parameter of the system. It is possible, that in another domain, the relation between these two variables might be the opposite.

To illustrate the aforementioned reasoning consider the well known system of thermal explosion in gaseous mixture with heat loss, which was analyzed for the first time by Semenov and at present it is called after him. The dynamical behaviour of this system is studied in detail and the interested reader is referred to publications \cite{17, 18, 16, 4}. The conventional form of the Semenov’s model \cite{37, 8} reads

\[
\frac{\gamma d\theta}{d\tau} = \eta \exp \left( \frac{\theta}{1 + \beta \theta} \right) - \delta \theta, \quad \theta(\tau = 0) = 0 \tag{7}
\]

\[
\frac{d\eta}{d\tau} = -\eta \exp \left( \frac{\theta}{1 + \beta \theta} \right), \quad \eta(\tau = 0) = 1 \tag{8}
\]

In the system \( (7) \)-(8), the following notations were used: \( \tau \) - dimensionless time, \( \theta \) - dimensionless temperature, \( \eta \) - dimensionless concentration, \( \delta \) is a dimensionless heat loss parameter, \( \gamma \) is a reciprocal of the dimensionless adiabatic temperature rise and \( \beta \) is a dimensionless ambient temperature. Parameters \( \beta \) and \( \gamma \) are the conventional parameters of Semenov’s theory of thermal explosion. Their characteristic values are small compared with unity for most gaseous mixtures due to the high exothermicity and activation energy of the chemical reaction. The exponential and linear (with respect to \( \theta \)) terms indicate heat release due to exothermic chemical reaction and heat loss to the ambient correspondingly.

In accordance with the reasoning presented in Section 3, the slow curve of the system \( (7) \)-(8) is given by the RHS of the Equation \( (7) \). The slow curve \textit{OTP} has an S-shape (see Figure 1, the second part of the S is not presented in the Figure). The equation for the slow curve
Figure 1. Various types of trajectories for the Semenov’s model of thermal explosion

has a unique isolate solution $\theta(\eta)$ for all $\eta$, except of the turning point $T$. The slow curve is divided by the turning point $T$ into the two parts: stable (attracting) parts ($OT$) and unstable (repelling) part ($TP$). The solution of the initial-value problem (7) - (8) starts from the initial point $I_i, i = 1, 2, 3$, which relative location (with respect to the slow curve) is determined by the parameter $\delta$.

Consider possible regimes of system dynamics along the lines of the present subsection. At the initial stage of the trajectories (close to the points $I_i, i = 1, 2, 3$, the variable $\theta$ is fast, whereas another one $\eta$ is slow. Hence, the trajectory here is characterized by the constant value of slow variable ($\eta = 1$) (concentration of the combustible reagent), in other words the trajectory moves parallel to the $\eta$-axes. Later the situation can change depending on the relative location of the initial point $I_i, i = 1, 2, 3$. The trajectory starting at the point $I_1$ after the initial stage of fast motion ($I_1U$) approaches the slow curve $OTP$. On the slow curve the relative rates of the processes are comparable, and the system dynamics is governed by the reduced system on the slow curve. One can see in Figure 1 that trajectory “adheres” to the slow part of the manifold and moves ($UO$) toward the singular point $O$. Another type of the trajectories is presented by starting point $I_3$. The trajectory starting at this point does not approaches the slow curve $OTP$. Asymptotically this type of motion (explosive trajectory) can continue for an infinitely long time. Nevertheless, for any finite value of the small parameter $\gamma$ the trajectory $I_3V$ approaches rather quickly the bound of the domain, where the hierarchy between the accepted variables exists. After that one need to take into account corrections of the fast motion. For some parameter value $\delta$, the unstable part of the slow curve ($TP$) is a part of the trajectory of the system (7) - (8), in the $O(\gamma)$ approximation. This trajectory is defined as critical because it separates the two main typical types of the trajectories: slow (non-explosive) ($I_1UO$) and explosive ($I_3V$). The critical trajectory ($I_2TV$) determines the critical value of the system parameter, i.e. the explosion limit. It is worth noting here, that the first term of this asymptotic expansion reproduces the well-known Semenov explosion limit. The critical trajectory determines also the maximum sub-critical temperature. Moreover it allows us to analyze transition from non-explosive regimes to explosive ones. For analysis of the case in more detail the reader is referred to the papers and books mentioned earlier.

4.2. Singularity Perturbed Vector Field - Possible Geometrical Interpretation (Simple Case)

Suppose now that we have not a-priori information concerning a presence of the small parameter (internal hidden hierarchy) in the given system of ODEs. The authors suggest a procedure, which allows us to uncover whether the given system can be treated as SPS. For simplicity let us start with the two-dimensional system (later all details of the proposed procedure can be easily generalized for an arbitrary dimension an initial system).
\[
\begin{align*}
\frac{dx}{dt} &= P(x, y) \\
\frac{dy}{dt} &= Q(x, y),
\end{align*}
\]  

where the functions \(P(x, y)\) and \(Q(x, y)\) determines some two-dimensional vector field (with an unknown relation between its components) within the domain \(W\) of interest. At the first step of the proposed procedure we suggest comparing the maximal values of these two functions within the considered domain and to determine the largest of the two. This function (suppose, the \(Q(x, y)\) has the largest value) represents a candidate for the fast component of the vector field, whereas the corresponding variable (\(y\)) serves as a candidate for the fast variable. As the result of this conclusion, at the second step we need to exclude from consideration some neighbourhood of the isocline of the function \(Q(x, y)\) (because of the evident fact, that this isocline represents a candidate for the slow manifold). As the third step we construct the function \(\zeta(x, y) = \frac{P(x, y)}{Q(x, y)}\) and look for \(\sup \zeta(x, y)\) within the rest of the initial domain of interest (similar to the algorithm, described above). Once we have the value of \(\zeta_0 = \sup \zeta(x, y)\) much smaller than unity, than it can be exploited as a global small parameter of the given system of ODEs and the system can be treated as an SPS. To re-write the system (9) - (10) in the standard form of an SPS, one can multiply the second equation (10) by the obtained small parameter \(\zeta_0\). The re-written system reads

\[
\begin{align*}
\frac{dx}{dt} &= P(x, y) \\
\zeta_0 \frac{dy}{dt} &= Q_1(x, y), \quad Q_1(x, y) = \zeta_0 Q(x, y),
\end{align*}
\]

where the RHSs of the both equations contain functions of the same order in accordance to the accepted definitions.

### 4.3. Singularly Perturbed Vector Field - Possible Geometrical Interpretation (General Case)

All the situations analyzed in the previous subsections 4.1, 4.2 had one common property: it was implicitly supposed that one of the coordinates (in the two-dimensional case) is fast, whereas the second one is slow. This situation is to some extent also an idealization. Suppose now, that we deal with the system of ODEs, where directions of the fast and slow motions are ”mixed”, that is none of the coordinates (not \(x\) neither \(y\)) can be recognized as pure fast or pure slow according to the algorithm, described in the previous subsection. The natural question may be formulated as follows: is it possible to determine the direction of the fast motion in a general case (when the desired direction does not coincide with one of the axes)? To supply a proper reply to the question, let us define the singular perturbed vector field (we will use this notion later). Consider the following system of ODEs (as in the previous case, it would be reasonable to start from the two-dimensional case, a corresponding generalization may be formulated later)

\[
\frac{dZ}{dt} = \Psi(Z, \epsilon), \quad \epsilon << 1
\]

where \(Z\) is a vector of variables, \(\epsilon\) is a small parameter. One can say that the vector field \(\Psi(Z, \epsilon)\) is singularly perturbed if there is a vector \(\vec{\sigma}\), so that the direction, obtained asymptotically \((\epsilon \to 0)\) from the original vector field \(\Psi(Z, \epsilon)\), and the direction \(\vec{\sigma}\) are parallel: \(\Psi(Z, \epsilon)_{\epsilon \to 0} \parallel \vec{\sigma}\). In another, less formal words, under additional assumption \(\epsilon \to 0\) the original vector field \(\Psi(Z, \epsilon)\) is reduced to another vector field of lower dimension (dimension of the straight line, parallel to the vector \(\vec{\sigma}\) is smaller by one than that of the original vector field \(\Psi(Z, \epsilon)\)). This low-dimensional vector field represents a manifold of fast motion. Note here that
this reduction of the original vector field is possible due to the fact that the small parameter \( \epsilon \) is explicit in the definition of the field (theoretical idealization).

The procedure described above can be easily generalized for the \( n \)-dimensional case. In this case, we can say that the vector field \( \Psi(Z, \epsilon) \) is a singular perturbed one if there is a \( m \)-dimensional subspace \( \Sigma \) of the original \( n \)-dimensional \((m < n)\) phase space, so that the vector field \( \Psi(Z, 0) \) (obtained asymptotically \((\epsilon \to 0)\) from the original vector field \( \Psi(Z, \epsilon) \)), is parallel to the subspace \( \Sigma \).

The aforementioned algorithm is applicable in the case, when the original system of ODEs contains the small parameter in the explicit form (and can tend to zero), similar to (13). It is obvious that it is not a general case and in any realistic situation a researcher needs to investigate a system of ODEs, where the question of a presence of the small parameter is open or/and demands separate cumbersome investigation.

5. General Framework of Local Approach

In this section we will introduce a general framework and examples of systems that can be represented locally and globally as a singularly perturbed system with the help of specially chosen matrix field. This field produces a new coordinate system in which the original system has singularly perturbed form.

The main motivation for this definition is the ILDM-method based on the matrix field defined by Jacoby matrices. According to the ILDM-method this matrix field is determined by basis of eigenvectors that can be generally subdivided into two parts ("fast" and "slow") depending on relevant eigenvalues according to the spectral gap and the original system can be rewritten in this basis as a SPS.

As we will see this cannot be realized properly by ILDM-method in very simple model examples. Therefore we will start with discussion of the ILDM-method that can be used as a basic numerical tool for investigating the local structure of a given vector field we will introduce a suggested improvement and then propose methods for the global analysis.

Let us now consider an arbitrary system of ODEs in a general autonomous form,

\[
\frac{dZ}{dt} = \Theta(Z),
\]

(14)

which, on one hand, is not written in the standard form of a SPS and, on the other hand, does not contain the small parameter in the explicit form. There are two possibilities: (i) the system is not multi-scale, (ii) the system has a gap in its characteristic scales (e.g., multi-scale) but the existing hierarchy is hidden.

If the system under consideration is not multi-scale (i), none of the asymptotic approaches can be applied to it.

The system with internal ("hidden") hierarchy (ii) is much more attractive for us both from a pure scientific and a practical points of view. The presence of the internal hierarchy can be interpreted, for example, as the existence of another pair of coordinates (in the two-dimensional case), where the original system of ODEs can be re-written in the form of the conventional SPS. The question, in turn, can be formulated as follows: is it possible to build an algorithm allowing us to find these new coordinates?

Generally the authors suggest an algorithm which improves the existing ILDM-method and able to answer the question in the simplest possible case. Namely, presume that a desired system of coordinates can be obtained from the original ones by a linear transformation (rotation). More complex cases are beyond the scope of the present manuscript.

Consider a two-dimensional version of the system (14), all our constructions for this case may be generalized for any multiple dimensional case. Any rotation of the original coordinates can be represented (locally) by an orthogonal matrix \( \tilde{Q} \). Thus, we are interested to obtain the matrix
of the transformation, which can transform the initial system (14) into the system written in the form of a SPS. In other words, the first equation of the transformed matrix is a fast equation, whereas the second one is slow, correspondingly. We can distinguish two distinct parts in the transformation matrix \( \tilde{Q} \). These two parts are responsible for the transformation into the new fast and slow variables, respectively. Hence, the matrix \( \tilde{Q} \) can be written in the following form:

\[
\tilde{Q} = \begin{pmatrix} Q_f \\ Q_s \end{pmatrix}
\]

(15)

where \( Q_f \) is a submatrix responsible for the transformation of the initial coordinates \( Z \) into the new fast coordinate \( X = \tilde{Q}_f Z \), and \( Q_s \) is a submatrix responsible for the transformation of the initial coordinates \( Z \) into the new slow coordinate \( Y = \tilde{Q}_s Z \). Then,

\[
\frac{dX}{dt} = F(X, Y) + \frac{dQ_f}{dt} Z, \quad F(X, Y) = \tilde{Q}_f \Theta(Z)
\]

(16)

\[
\frac{dY}{dt} = G(X, Y) + \frac{dQ_s}{dt} Z, \quad G(X, Y) = \tilde{Q}_s \Theta(Z)
\]

(17)

To single out the slow and the fast parts of the vector field, one needs to find a transformation matrix \( \tilde{Q} \) so that the derivatives of the matrix will be essentially smaller than the existing vector field. This condition can be written in the form

\[
\|F(X, Y)\| >> \left\| \frac{dQ_f}{dt} Z \right\| \quad (18)
\]

\[
\|G(X, Y)\| >> \left\| \frac{dQ_s}{dt} Z \right\| \quad (19)
\]

Once this condition is fulfilled, the system (16)-(17) can be re-written in the approximate form close to the form of a SPS

\[
\frac{dX}{dt} = F(X, Y),
\]

(20)

\[
\frac{dY}{dt} = G(X, Y),
\]

(21)

The present form of the system is identical to one considered in the Section 4. Hence, starting from this point all subsequent analyse can be repeated. The traditional idea of introducing new nonlinear coordinates that convert the original system into a singularly perturbed one is also relevant in the context of this section, because any nonlinear change of variable procedure produces a matrix field of the necessary type.

It would be worthwhile to note here that there is an infinite number of possible transformations of the initial system of coordinates and the procedure described above does not suggest any specific type of transformation. The choice depends on the type of the specific problem under consideration and the nature of the gap between distinct time scales.

5.1. Suggested approach - TILDM

ILDM was originally constructed to numerically handle systems of ODEs containing a large number of equations. The method has proved to be an efficient tool for the simplification of detailed chemical kinetics [26, 27, 6, 4, 22, 32, 33, 34, 39, 9].
Let us explain shortly the main idea of the suggested modification of the ILDM method (which can be called TILDM) on the simple two-dimensional case (we will the meaning of the letter T).

As it was pointed out the ILDM-method uses the local Jacobian eigenspaces, more precisely the Shur basis for local Jacobian matrix, as the transformation of coordinates. It is obvious that locally the best linear approximation of the vector field is the Jacobian matrix, but let us firstly consider two linear examples, which demonstrate that even for singularly perturbed systems a division into fast and slow eigenvectors not necessary exists.

Let us start form a simplest possible nontrivial case of the system (Linear Example LE1)

\[
\begin{align*}
\frac{dx}{dt} &= -x - \frac{1}{\epsilon} y, \\
\frac{dy}{dt} &= -y,
\end{align*}
\]

(22) (23)

It is obvious, that the Jacobian of the considered system equals the matrix \( A \) of the RHS of the system (22) - (23). Eigenvalues of the matrix \( A \) are real and equal (minus unity). According to the traditional interpretation of the ILDM approach, there is no internal hierarchy in the considered system (22) - (23) and the analysis can not proceed further. Nevertheless, as one can readily see, the original system (22) - (23) has essentially different rates of change (at least in the region, where the functions \( x(t) \) and \( y(t) \) are of the same order: within this domain \( x(t) \) is fast and \( y(t) \) is slow). Moreover, multiplying by \( \epsilon \), we can re-write the first equation in the conventional SPS form

\[
\begin{align*}
\epsilon \frac{dx}{dt} &= \Theta_f(x, y), & \Theta_f(x, y) &= -\epsilon x - y, \\
\frac{dy}{dt} &= \Theta_s(x, y), & \Theta_s(x, y) &= -y,
\end{align*}
\]

(24) (25)

This leads us to the conclusion that even in the simplest linear cases with strongly determined hierarchy the eigenvalues of the Jacobian do not always provide us with correct information regarding possible reduction to singularly perturbed form.

It would be worthwhile also to consider the system with complex eigenvalues (Linear Example LE2)

\[
\begin{align*}
\frac{dx}{dt} &= x - \frac{1}{\epsilon} y, \\
\frac{dy}{dt} &= x + y,
\end{align*}
\]

(26) (27)

The main idea of this two-dimensional example is to demonstrate a drawback of the ILDM approach in the case of complex eigenvalues of a corresponding Jacoby matrix. Similar to (22) - (23), the system (26) - (27) can be easily written in the conventional form of the SPS. Nevertheless, the ILDM method cannot indicate the existing hierarchy because the real parts of the two complex eigenvalues are equal

\[
\lambda_{1,2} = 1 \pm \frac{i}{\sqrt{\epsilon}} + O(\epsilon),
\]

(28)

and, therefore, according to the standard ILDM approach, there is no distinction in rates of change of the two processes. In geometrical language, the traditional ILDM procedure fails to decompose the vector field \((Z)\) (determined by the RHS of the system (26) - (27)) into fast and slow components. This unexpected result looks a bit confusing, especially in the light of the evident decomposition of the original vector field into the fast and slow components.
\[
\frac{dx}{dt} = \Theta_f(x, y), \quad \Theta_f(x, y) = \epsilon x - y, \quad (29)
\]

\[
\frac{dy}{dt} = \Theta_s(x, y), \quad \Theta_s(x, y) = x + y, \quad (30)
\]

It is not hard to see that in both examples (LE1 and LE2) the Jacobian matrix, which coincides with vector field, does not provide a hierarchy. Assuming that there is a linear mapping, the information about its eigenspaces may be insufficient to evaluation of the ”hidden” hierarchical structure.

It would be ideal, if we could build a transformation, which converts the original coordinates (variables) into these fast and slow directions. The latter can be found by using the fact that an arbitrary linear transformation (mapping) maps the unit sphere with the center in the origin to a hyperellipsoid.

Hence, we can identify the directions of the fast and slow motions with directions of the large and small semi-axes of the ellipsoid, respectively. To build the desired transformation consider a matrix \( M \) of an arbitrary linear transformation and its transpose matrix \( M^* \). The eigenvalues of the matrix \( MM^* \) represent the square length of the ellipse’s semi axes and corresponding eigenvectors coincide with the directions of the semi axes. One of the distinguishing features of the matrix of the type \( MM^* \) is an absence of complex eigenvalues (all eigenvalues are real and corresponding eigenvectors are orthogonal). Therefore, assuming that the Jacobian \( J \) of the considered system contains the relevant information regarding system dynamics (hierarchy of the system), we can conclude that the matrix of the transformation chosen as \( JJ^* \) provides us with more accurate information regarding decomposition that the Jacobian \( J \) does.

To summarize these reasonings and to transform the explained idea into a formal procedure let us describe here very briefly the essential analytical steps of the TILDM-manifold construction (for the system (14), for example) following the same scheme as for ILDM case (note, that the main purpose of the TILDM procedure coincides with that of the ILDM: to determine the ”fast” and ”slow” subspaces and to construct the corresponding TILDM manifold for the system (14)).

For an arbitrary point \( Z \):

1. Build matrix \( T(Z) = J(Z)J^*(Z) \) and determine its eigenvalues \( \lambda_i \) \( (i = 1, 2, ..., n) \).
2. Check whether a splitting exists (its absence means that the suggested procedure is inapplicable). If ”Yes”, re-order the obtained eigenvalues as follows
   \[ \lambda_i \gg \tau > \lambda_j, \quad i = 1, ..., n_f, \quad j = n_f + 1, n_f + 2, ..., n. \]
3. Build matrices \( Q(Z) \) and \( \tilde{Q}(Z) = Q^{-1}(Z) \) along the conventional rules used in ILDM approach

\[
\tilde{Q}(Z) = Q^{-1}(Z) = \left( \begin{array}{c} \tilde{Q}_f(Z) \\ \tilde{Q}_s(Z) \end{array} \right)
\]

4. Obtain a system of equations \( \tilde{Q}_f(Z) \cdot \Theta(Z) = 0 \) describing the TILDM manifold.

To illustrate the efficiency of the proposed algorithm, let us apply TILDM to the linear examples, considered earlier. Start with the system (22) - (23) (LE1). The eigenvalues of the matrix \( JJ^* \) read as follows

\[
\lambda_1 = \frac{1}{\epsilon^2} + 2 + O(\epsilon^2), \quad \lambda_2 = O(\epsilon^2)
\]

Therefore, the corresponding transformation matrix can be presented in the following form (terms of only the leading order are written, terms of the order \( O(\epsilon^2) \) are neglected, vectors are normalized)
\[
\dot{\mathbf{Q}} = \begin{pmatrix}
\tilde{Q}_f(Z) \\
\tilde{Q}_s(Z)
\end{pmatrix} = \begin{pmatrix}
1 & \varepsilon \\
-\varepsilon & 1
\end{pmatrix}
\] (33)

It can be readily seen that the eigenvectors corresponding to the eigenvalues (32) coincide with the corresponding directions of the fast and slow motions: the eigenvector \(\tilde{Q}_f\) (the first row of the matrix \(\mathbf{Q}\) - see Equation (33)) is asymptotically close to the direction of the fast motion (parallel to the \(x\)-axes), whereas the eigenvector \(\tilde{Q}_s\) (the second row of the matrix \(\mathbf{Q}\)) is orthogonal to \(\tilde{Q}_f\).

The aforementioned formalized algorithm needs some comments. Due to the above stated a property of the symmetric matrix, the transformation matrix \(T(Z) = J(Z)J^{\ast}(Z)\) has no complex eigenvalues. This means, that we are able to establish a relation between the processes involved in the whole phase space (and not in the region only, where the eigenvalues of the Jacobian are real, as in the conventional ILDM procedure).

On the other hand, this evident advantage has its own drawback - all eigenvalues are positive, i.e. information regarding the stability of the corresponding parts of the unknown manifolds is lost. Nevertheless, an analysis of the stability can be performed on the basis of the suitable analysis of the Jacoby matrix \(J\) at any point \(Z_0\) that belongs to TILDM-manifold. Once a spectrum of \(\tilde{Q}_f(Z_0) \cdot J \cdot \tilde{Q}_f(Z_0)\) has negative real parts, we can deduce that the corresponding TILDM manifold is stable. In any other case the corresponding TILDM manifolds is unstable. Remark regarding necessary smallness of the variations of the matrix field \(Q\) still remains crucial for TILDM as well as for ILDM.

5.2. TILDM - application

Here we consider a mathematical model of the ignition of a cold fuel spray in a hot combustible mixture. A formulation of the physical model and detailed asymptotic analysis of the dynamics of the corresponding system of governing equations along the lines of the MIM approach can be found in the paper [3]. The relevant data were taken from [40]. The reduced system of ODEs contains two equations and reads

\[
\gamma \frac{du}{d\tau} = (\eta(u, r))^{\eta}(\xi(u, r))^{b} \exp \left( \frac{u}{1 + \beta u} \right) - \varepsilon_1 r(u + \theta_0) = F_2(u, r), \quad u(0) = 0,
\] (34)

\[
\varepsilon \frac{dr^3}{d\tau} = -\varepsilon_1 r(u + \theta_0), \quad r(0) = 1,
\] (35)

\[
\eta(u, r) = \eta_0 - \frac{\gamma u - \varepsilon_2(\nu_{fu}\psi - 1)(1 - r^3)}{\nu_{fu}}, \quad \xi(u, r) = 1 - \frac{\gamma u + \varepsilon_2(1 - r^3)}{\nu_{ox}},
\] (36)

Here \(u\) is a dimensionless temperature, \(\eta, \xi\) are dimensionless concentrations of the fuel and oxidizer, respectively, \(r\) is droplet radius, \(\gamma\) is a reciprocal of the dimensionless adiabatic temperature rise and \(\beta\) is a dimensionless initial temperature. The parameters \(\gamma, \beta\) are normally small with respect to unity. The parameter \(\gamma\) serves as the singular parameter of the system. The value of the parameter \(\varepsilon_2\) can essentially vary and it can serve as a singular perturbation parameter too.

Therefore, the system (34)-(35) can be treated as a multi-scale system. Unlike the Semenov’s model, the system (34)-(35) has two small parameters and fast-slow relation depends on the value of the ratio \(\gamma/\varepsilon_2\). Let us restrict ourselves to the case of fast temperature \((\gamma/\varepsilon_2 << 1)\). Assuming this, the slow curve \(F_2(u, r) = 0\) of the system (34)-(35) is given [11] by , where the system parameters for the example presented here looks \(\beta = 0.04, \gamma = 0.001, \varepsilon_1 = 1, \varepsilon_2 = 0.1, \psi = 15, \nu_{fu} = 0.127, \nu_{ox} = 0.327, a = 0.25, b = 1.5, \theta_0 = 1.5, \eta_0 = 0.25\). The slow curve
Figure 2. Application of the TILDM approach to the system (34)-(35). TILDM manifold is depicted as bold dashed line, the slow curve $\Omega_2$ - thin solid line, a sample numerical trajectory starting from $I - IABDC$, the bold dotted line.

$\Omega_2$ can be readily obtained by solving the equation $F_2(u, r) = 0$, whereas the equations for the ILDM as well as for the TILDM are solved numerically.

The Figures 2 - 4 present results of the analysis in a graphical form. Figure 2 depicts the TILDM manifold (bold dashed line), the slow curve $\Omega_2$ (thin solid line) and a sample numerical trajectory starting from $I$ ($IABDC$, the bold dotted line). One can see, that the TILDM manifold and the slow curve almost coincide. One can readily see that the trajectory starts at the point $I(0, 1)$ and moves fast towards the attractive branch $AT$ of the manifold. During this first fast stage the slow variable ($r$) preserves its initial value ($r = 1$). At the intersection point $A$ the relative rates of the processes involved become comparable and the trajectory begins its slow stage ($AB$, along the slow curve). In the vicinity of the turning point $T$ the stable branch of the slow curve loses attraction of trajectories, the trajectory tears off and the second fast stage begins ($BDC$, final thermal explosion).

The ILDM technique yields a much richer picture, which should be additionally analysed (Fig.3). For our purposes, we depict two curves built on the basis of the two eigenvalues of the Jacobian. The curve $ABGR$ corresponds to the smaller eigenvalue $\lambda_1$, whereas the curve $FJK$ - to the second one $\lambda_2$. The part $AB$ of the ILDM manifold approximates the stable branch of the slow curve/TILDM and, in fact, represents the single desired result of the ILDM machinery. To understand the whole picture, we need to study the behaviour of the Jacobian’s eigenvalues. The curve $GEF$ distinguishes the regions of the negative (left) and positive (right) values of the $\lambda_1$ ($\lambda_2$ is positive in the chosen region), therefore the ILDM technique is not applicable right of the curve $GEF$. Moreover, the ILDM machinery demands the existence of splitting of the processes involved (essential difference in rates of change). The curve $VW$ presents the set of points where the ratio $|\lambda_1/\lambda_2| = 10$ is valid. We can see that left to the curve $VW$ the ILDM manifold approximates the slow curve quite well, whereas to the right of this curve the ILDM manifold ($ABGR$) begins to move away from the real trajectory ($ABDC$). This can be explained by the fact that the relation between the eigenvalues decreases from 10 (on the curve $VW$) to the region of unity and less and this makes the application of the ILDM technique invalid.

Additional information on the dynamical picture of the system (34)-(35) can be obtained
Figure 3. Application of the ILDM approach to the system (34)-(35).

from Fig.4, which presents both the relevant curves and the trajectories. Figure 4 depicts the slow curve $\Omega_2$ (solid line $ABTF$), TILDM (circles, $ABTF$), ILDM (solid lines $ABGG$ and $KJF$), nuances of the gray colors correspond to different values of the Jacobian’s eigenvalue $\lambda_1$. One can easily see that the trajectories are attracted to the branch $AB$, whereas the branch $TF$ of the slow curve/TILDM is repulsive and the trajectories are rejected from it. Moreover, as we saw in the Fig.3, in the region where $\lambda_1$ becomes positive, the curve $BGR$ loses its critical feature.

One can easily see that the suggested modification (TILDM) of the existing algorithm (ILDM) successfully overcomes main problems, which were uncovered during the analysis performed by the authors.

Figure 4. Application of the ILDM approach to the system (34)-(35).
5.3. Dynamic Decomposition Method

As it was mentioned above, both fast and slow motions can represent a subject of interest in various industrial applications. There is a number of models, where the fast stage of the system dynamics attracts the main part of the researcher’s attention. In this Subsection we will illustrate the aforementioned theoretical reasoning (see previous Section) by real-world applications of modelling combustion of diesel engine fuel.

It is well known that numerical approach (CFD codes) is one of the most popular tools in modelling fuel spray dynamics. Numerical spray modelling is traditionally based on the Lagrangian approach coupled with the Eulerian representation of the gas phase. This permits the decomposition of complicated and highly nonlinear systems of PDEs, describing interactions between computational cells, and the systems of ODEs that govern processes in individual computational cells, including liquid/gas phase exchange and chemical kinetics. The systems of ODEs are usually integrated using much shorter time steps $dt$ (typically $ms$) than the global time steps used for calculating the gas phase $\delta t$ (typically 10 $ms$). Thus the decomposition of ODEs and PDEs is de-facto used.

Further decomposition of the system of ODEs, describing droplets dynamics inside individual computational cells, is widely used also. The simplest decomposition of this system of ODEs is based on the sequential solution of individual subsystems comprising this system (split operator approach). In this approach, the solution of each individual subsystem for a given subset of variables is based on the assumption that all the other variables are fixed. The sequence of solving individual subsystems is often chosen rather arbitrarily and the results sometimes vary substantially depending on the order in which these subsystems are solved. In the case of a multiscale system, the reliability of this approach becomes altogether questionable. To overcome these problems the multi-scale nature of ODEs needs to be investigated before any attempt to solve them is made.

A number of approaches for system decomposition into lower dimension subsystems (ILDM, CSP) were developed with a view of application to modelling chemical kinetics. There are many similarities between these methods. They are based on a rigorous scale separation such that ‘fast’ and ‘slow’ subspaces of the chemical source term are defined and mechanisms of much reduced stiffness are constructed. Their generalization to general CFD codes has not been considered to the best of our knowledge.

The existing approaches to decomposing systems of ODEs were developed and investigated with a view to application to rather special problems, and were based on a number of assumptions. These include fixing the decomposition over the whole period of the process, and not allowing its hierarchy to change with time. The underlying philosophy of these approaches, however, seems to be attractive for application to the analysis in a wide range of physical and engineering problems including spray modelling in general computational fluid dynamics (CFD) codes.

A novel decomposition technique for a system of ordinary differential equations was suggested by the authors (Bykov et al, submitted), based on the geometrical version of the integral manifold method (MIM). This technique is based on comparing the values of the right hand sides of these equations, leading to the separation of the equations into ”fast” and ”slow” variables. The hierarchy of the decomposition is allowed to vary with time. This approach overcomes some of the problems of the existing methods and is, essentially, focused on the fast stage of the system’s dynamics. In particular, the proposed technique allows the change of the nature of decomposition with time (dynamic decomposition).

As in the original integral manifold method, the developed approach to decomposition of the system of ODEs is based on the division of system variables into ”fast” and ”slow”. The point is that this subdivision is performed on every global time step and in every computational cell (the hierarchy can change from step to step and from cell to cell). Therefore, the aforementioned...
subdivision is performed an enormous number of times during the single calculation of the initial system of PDEs and any approximation can essentially reduce the time.

In contrast to the original version of the integral manifold method, linearised variations of slow variables during time evolution of the fast variables will be taken into account as the first order approximation to the fast manifold. The usefulness of this division depends on whether the ‘fast’ subsystem has a lower dimension compared with the ‘slow’ subsystem. The procedure can be iterative and result in a hierarchical division of the original system. For example the ‘slow’ subsystem can, in turn, be subdivided into ‘slow’ and ‘very slow’ subsystems.

To explain the main idea of the proposed approach (which can be conditionally called dynamic decomposition technique), the essence of the algorithm may be very shortly formulated as follows: (1) asymptotic analysis of the given system of ODEs (comparison of the RHSs of the governing equations); (2) once one concludes that there is a gap in time scales, the original system is re-ordered (as a result one obtains system in conventional SPS form with small, but finite parameter); (3) a calculation is performed for the fast part of the re-ordered system; (4) correction of the approximate fast motion is performed (fast manifold). To demonstrate how the scheme is realized, let us consider the system, the state of which is characterized by dimensionless parameters, which are denoted as $Z_n$ ($n = 1, 2, \ldots, n$). The value of each of these parameters anywhere in space depends on time $t$, i.e. $Z_n = Z_n(t)$. This dependence can be found from the solution of the system of equations, which can be presented in a vector form:

$$\frac{dZ}{dt} = \Phi(Z),$$

where:

$$Z = (Z_1, Z_2, \ldots, Z_n), \quad \Phi = (\Phi_1, \Phi_2, \ldots, \Phi_n).$$

In the general case, a rigorous coupled numerical solution could be found. As we will see further, the suggested approach (based on reducing the dimensions of this system is much more practical. This could be based on organizing Equations (37) in terms of decreasing parameters $Y_i$:

$$Y_i = \frac{\Phi_i(t_k)}{Z_i(t_k)},$$

where $\Phi_i(t_k) \equiv \Phi_{ik} \equiv \Phi_i(Z_1(t_k), Z_2(t_k), \ldots, Z_i(t_k), \ldots, Z_n(t_k))$ and $Z_i(t_k) \equiv Z_{ik}$ are the right hand sides of Equations (37) and the values of $Z_i$ taken at time $t_k$ for time step: $\Delta t : t_k \rightarrow t_{k+1}$, $i = 1, 2, \ldots, n$. For $Z_{ik}$ close to zero we have a special case which requires additional investigation. In practice, in most cases we can just assume that $Z_{ik}$ is a large number.

If $Y_i$ is greater than a certain $a priori$ chosen positive number $\alpha < 1$, then the corresponding equation can be considered fast and this should be solved rigorously. If the number of ‘fast’ equations is $f \neq 0$, then the system is called multi-scale and this procedure effectively reduces the dimension of the system (37) from $n$ to $f$. This dimension reduction is particularly attractive when $f$ is small (1 or 2). The procedure described allows us to perform subdivision of the ODEs to be solved into fast and slow ones on every time step and within every cell of the mesh. This, in turn, permits us to conduct an asymptotic analysis (with user-defined small parameter).

In the suggested approach, we reorganize $Y_i$ in descending order as:

$$Y_{i_1} \geq Y_{i_2} \geq \ldots \geq Y_{i_j} \geq \ldots \geq Y_{i_n}. \quad (39)$$

If we are able to find $j = f$ such that

$$\frac{Y_{i_{f+1}}}{Y_{i_f}} < \epsilon, \quad (40)$$
where $\epsilon$ is another a priori chosen small parameter, then we can conclude that the system can be decomposed locally ($\Delta t : t_k \rightarrow t_{k+1}$) into two subsystems: ‘fast’ and ‘slow’. Note that the subscript $i_j$ indicates the order in which the parameters are organized (no summation over $f$ takes place).

Having introduced a new small positive parameter $\epsilon \ll 1$ and remembering the definitions of $Q_f$ and $Q_s$, we can rewrite the system (37) in a form, where its two parts are separated (as in MIM):

$$
\frac{dU}{dt} = \epsilon Q_f^{-1}(Z_0) \Phi \left( Q(Z_0) \begin{pmatrix} U \\ V \end{pmatrix} \right) \equiv \Phi_{f\epsilon} \left( \begin{pmatrix} U \\ V \end{pmatrix} \right),
$$

(41)

$$
\frac{dV}{dt} = Q_s^{-1}(Z_0) \Phi \left( Q(Z_0) \begin{pmatrix} U \\ V \end{pmatrix} \right) \equiv \Phi_s \left( \begin{pmatrix} U \\ V \end{pmatrix} \right),
$$

(42)

where $\Phi_{f\epsilon} = \epsilon \Phi_f$, $Q$ is simply reordering matrix such that first $N_f$ correspond to relatively fast variables and the next $N_S$ variables are relatively slow. In this presentation the right hand sides of (41) and (42) are expected to be of the same order of magnitude over the specified period (time step).

Equations (41) and (42) will be integrated over the time period $\Delta t : t_k \rightarrow t_{k+1}$. The zeroth order solution of Equation (42) is just a constant value of the slow variable: $V^{0}_{k+1} = V_k = ((Z_{i_f+1}^k, \ldots, Z_{i_n}^k), \ldots, (Z_{i_f+1}^k, \ldots, Z_{i_n}^k)$, where the superscript 0 indicates the zeroth approximation, while the subscripts $k$ and $k+1$ indicate time. The zeroth order for the fast variable is found from (41) with $V = V_k$. This could be interpreted as the equation for the slow variable on the fast manifold. This means that Equation (41) is approximated by the following system:

$$
\frac{dU}{dt} = \Phi_f \left( \begin{pmatrix} U \\ V_k \end{pmatrix} \right).
$$

(43)

The solution of (43) at $t = t_{k+1}$ ($U^{0}_{k+1}$) is the zeroth order approximation of the fast motion on the fast manifold at $t = t_k$. Note that the system (43) can be stiff in the general case, but with a reduced level of stiffness, compared with the original system (37). Hence, the suggested method is expected to reduce the level of stiffness of the system, but not to eliminate stiffness altogether.

Under the same zeroth order approximation the slow variables would remain constant over the same time step (see the previous Section). This, however, might lead to an unphysical result when slow variables would remain constant for any time $t > t_0$. Hence, one needs to calculate slow variables using at least the first order approximation. When $\epsilon$ is not asymptotically small, further, or higher order, approximations need to be considered. In this case we can introduce the new time scale $\tau = 1/\epsilon$ and write the expression for the value of $V(t_{k+1}) \equiv V_{k+1}$ in the form:

$$
V_{k+1} = V^{(0)}_{k} + \Phi_s \left( \begin{pmatrix} U^{(0)}_{k+1} \\ V^{(0)}_{k} \end{pmatrix} \right) \Delta t
$$

$$
= (Z_{i_f+1}^k + \Phi_{i_f+1} \left( U^{(0)}_{k+1}, V^{(0)}_{k} \right) \Delta t, \ldots, Z_{i_n}^k + \Phi_{i_f+1} \left( U^{(0)}_{k+1}, V^{(0)}_{k} \right) \Delta t.
$$

(44)

To increase accuracy of calculations one could continue the process to take into account the first order solution for the fast motion. Then the second order solution for the slow motion could be obtained etc.

The procedure described above was applied to spray combustion modelling. The mathematical model represents a system of 10 governing ODES: three basic equations - temperature ($T_d$) and radius ($R_d$) - for every one of the chosen three fractions ($i = 1, 2, 3$) (droplets with distinct radii $R_{di}$), and closing equations for the fuel vapour concentration $C_{fu}$.
oxygen concentration $C_{ox}$, temperature of the gas ($T_g$)) and pressure of the gas $P$. Hence, $Z = Z(T_{di}, R_{di}, C_{fu}, C_{ox}, T_g, \ldots)$. During every step the system is decomposed into fast and slow subsystems (note that ‘fast’ and ‘slow’ decomposition can be different for different phase space regions and on the distinct global time steps). Equations for fast variables are solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. The solution of the equations for the slow variables is presented in a simplified form, assuming linearised variation of these variables for the known time evolution of the fast variables. This can be considered as the first order approximation for the fast manifold.

![Figure 5. Number of solved equations vs time](image-url)

The efficiency of the suggested approach can be illustrated, by the total number of equations solved (the number of equations for fast variables could change with time). The corresponding plots of the numbers of equations are shown in Fig. 5. As follows from this figure, initially all 10 equations were solved, when the conventional approach was used. This number was reduced to 8 when the smallest droplet evaporated, and to 6 when two smallest droplets evaporated. Initially, the number fast variables to be solved was equal to 4, then it dropped to just one equation describing fuel vapour density. Between about 0.25 ms and 0.5 ms the number of equations for fast variables was equal to two (equations for fuel vapour density and the radius of the smallest droplet). Then again just the equation for fuel density was solved. Between about 0.6 ms and 0.8 ms the number of fast equations to be solved is comparable with the total number of equations solved. During this period the decomposition of the system is not useful. After about 0.8 ms and until about 1.8 ms only one equation (fuel density) or two equations (fuel density and the radius of the second droplet) were used.

To compare the CPU efficiency of the new (dynamic decomposition) and conventional CFD approaches, a series of runs for various time steps were performed. A polydisperse spray including three droplet parcels, was injected at the start of the calculation. For fixed time steps the CPU requirements of both conventional approaches were about the same. However, the accuracy of the suggested approach was always higher than that of the conventional approach. Thus the comparison of CPU requirements of both methods for fixed time steps would be misleading. An alternative approach needs to take into account the accuracy of calculations. As followed from our calculations, the autoignition delays predicted by the dynamic decomposition approach
coincided with those predicted by the full coupled solution for the time step of $\mu s$. This value of the autoignition delay was considered as the true value for further comparisons. For example, for the second set of parameters errors less than 1.5% were achieved for time step of $1.3 \cdot 10^{-5}$ s for the conventional CFD approach, and for time step of $2.4 \cdot 10^{-5}$ s for the new approach. When this effect was taken into account then, the CPU time for the new method was always smaller than that for the conventional approach. In some cases, the CPU reduction for the new approach was as high as factor of 3.

To recap this subsection, it would be worthwhile to underline that clear advantages of the suggested approach are demonstrated from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes. The difference between the solution of the full system of equations and the solution of the decomposed system of equations is shown to be negligibly small for practical applications.

6. Quasilinearization - Global Approach
In the previous Section an approximation of fast motion was suggested and its application was demonstrated. The approximation was build on comparison between coordinate functions of the original vector field (RHSs of corresponding governing equations). This type of the comparison produces a zero approximation of fast manifolds for the considered dynamic systems in the case when the system under consideration represents SPS in the phase space coordinates. Additionally, this comparison procedure permits us to renormalize RHSs of governing equations, so that after renormalization the systems had a standard SPS form with an explicit small parameter. The evident advantage of the this form is the fact that the system be easily subdivided into fast and slow subsystems.

The methods discussed above (ILDM, TILDM and their possible modifications) focus on a numerical evaluation of slow stable invariant manifolds for dynamical systems that are not obligatory SPSs for original coordinates but can be transformed (locally) into SPS with help of corresponding new local coordinate systems. These methods are efficient only in a small vicinity of slow stable invariant manifolds, because only in this case a Jacoby matrix $J$ of an original vector field contains information about the fast/slow subdivision.

It is not hard to understand that all methods mentioned have a local nature either by construction restrictions like in fast motion integration in CFD modeling (Subsection 5.3 or by using slow dynamics only (ILDM-like techniques) and can not be useful in reducing of the system dimension in a global sense. Namely, these methods are not able to decompose and describe correctly both fast and slow system dynamics simultaneously.

In the present Section we suggest a novel approach to build a global (which is valid for some bounded domain) transformation of the initial coordinates, which should allow us to transform the original system of ODEs into a conventional SPS form. According to the meaning of the adjective ”global” this transformation should be the same for the chosen domain and this is the principal distinction of this approach from the techniques considered and suggested earlier. We call these approximations (one can easily see that there is an infinite number of them) - global quasi-linearizations (GQL). The quasi-linearizations can be only useful for special parametric domains and comparatively simple vector fields. Fortunately, a lot of practical situations of real practical interest exist, where these approximations are applicable.

Suppose an arbitrary dynamical system can be potentially transformed into a singularly perturbed system by an appropriate choice of new coordinate system (the ”hidden” hierarchy exists). Assume also, that this transformation(s) is valid for any point within some bounded domain. Once the system meets these requirements - how can one find this transformation(s)?
6.1. Method of Global Quasilinearization

Let us return to the problem under consideration: how to construct a linear mapping to transform an original system of ODEs into SPS? It follows from the previous discussion that a Jacoby matrix of an arbitrary vector field cannot be of any help in general case here. Figure 6 gives a schematic illustration of different linear approximations for highly non-linear systems in a comparatively large domain of phase space. One can easily see that the two local approximations \( T_1 \) at points \( Z_1 \) and \( T_2 \) at \( Z_2 \) are essentially distinct and no one of them can serve as global for the whole domain. On the other hand, some global approximation \( T \) (straight dashed line in Figure 6) represents linearization, which can be determined as too ”rough” (the last statement demands an exact determination of ”roughness”). It is evident, that ideally, a local analysis of the considered system has to be combined with a global one.

![Figure 6](image_url)

**Figure 6.** Sketch for two different local linear approximations of the original vector field \( \Theta \) (thick solid curve), \( T_1 \) at points \( Z_1 \) and \( T_2 \) at \( Z_2 \) and some global approximation \( T \) is shown by the straight dashed line.

In this Section we suggest a way to construct the linear transformation that gives a desired representation globally. This transformation is based on the appropriate linear approximation \( T \) of an original vector field \( \Theta(Z) \) (in a new coordinate system the original system can be subdivided into ”fast - slow” subsystems in the whole domain of interest).

Let us return once again to equation (14) in a bounded domain of interest \( \Omega \):

\[
\frac{dZ}{dt} = \Theta(Z), \quad Z(t_0) = Z_0, \quad Z \in \Omega, \quad (45)
\]

General assumptions can be formulated as follows: we assume that within the domain a gap of time scale of subprocesses exists but it is hidden because of a non-appropriate coordinate system. This allows us to suggest that there exists a system of coordinates for which the system of ODEs (45) can be re-written in the conventional SPS form (1)-(2).

Ideally, this desired system of new coordinates should have a number \( n_s \) of coordinates, which directions represent the slow motion, and others coordinates represent \( n_s = n - n_f \) directions of fast motions.

Of course the possible constructions of the linear mapping \( T \) are very flexible and depend on an analytical nature of the vector field \( \Theta(Z) \). This dependence is a subject for a corresponding ”calculus”. Here we plan to discuss some general constructions.

Additionally, suppose we have already constructed such a linear approximation and consequently a representation of the system in the SPS form then there is the possibility to improve the approximations by considering/adding high order terms according to the general MIM theory, finding a first order approximation for an invariant manifold, second order and so on. Moreover, it could be done in both an implicit and explicit manner, but this is the issue
for further work and investigation. Technically, it is not a simple procedure, but fortunately in many applications a zero order approximation almost always give reasonable accuracy. Now, when we have a general structure of approximations of fast and slow motions developed in previous sections, we can introduce details of the proposed global approach.

The general idea of a global linear approximation $T$ of the vector fields $\Theta$ is very simple. Formally any vector field $\Theta(Z)$ is a nonlinear transformation (mapping) of its domain of definition $\Omega$ onto a subset of Euclidian space $U$. Choose $n + 1$ linearly independent points $Z_1, Z_2, ..., Z_{n+1}$ in $\Omega$. In any reasonable physical application the origin of coordinates $0$ belongs to $\Omega$ and the value $\Theta(0)$ is close to zero. Hence we can suppose that $Z_1 = 0$. The transformation $\Theta$ maps this set of $n + 1$ linearly independent points onto $n + 1$ points $V_1, V_2, ..., V_{n+1}$ of $U$. Almost without loss of accuracy we can suppose that $V_1 = 0$. There exists the unique linear transformation $T$ that transforms $Z_i$ in $V_i$, $i = 1, 2, ..., n$. The constructed linear approximation $T$ depends on the choice of $n + 1$ points $Z_1, Z_2, ..., Z_{n+1}$ in $\Omega$. Intuitively, this approximation will be global if these points are far from one another and will be more local if these points are close to each. The main problem for this approximation is an appropriate choice of a "typical" set of $n + 1$-points. Some kind of "infinitesimal construction" is also possible. We will call such kind of approximations as quasi-linearizations (QL).

Let us be a bit more precise and formal. A quasi-linearization $T$ of the vector field $\Theta$ can be constructed and applied in the following formal way:

1. The origin is transformed to the origin.

2. Choose $n$ linearly independent points $Z_1, Z_2, ..., Z_n$ in $\Omega$ such that the vector field $\Theta$ has a "typical" behavior of these points. These points can not be singular or close to singular points of the vector fields, and can not belong to invariant manifolds and can not be close to these manifolds. Of course this information is unknown a-priori, but for practical problems such choice does not represent serious problems.

3. Construct the unique linear mapping $T$ that transforms $Z_1, Z_2, ..., Z_n$ into $\Theta(Z_1), \Theta(Z_2), ..., \Theta(Z_n)$.

4. Evaluate eigenvalues of the matrix $TT^*$ (we use the same notation for the linear mapping $T$ and its matrix). Remember that the matrix $TT^*$ is symmetric and its eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ are real positive numbers. If $B$ is a unit sphere in $\mathbb{R}^n$ then $T(B)$ is an ellipsoid which semi-axes are square roots of $\lambda_1, \lambda_2, ..., \lambda_n$.

5. Organize the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ into two groups: big eigenvalues $\lambda_1, \lambda_2, ..., \lambda_{n_f}$ that correspond to directions of fast motions and small eigenvalues $\lambda_1, \lambda_2, ..., \lambda_{n_s}$ that correspond to directions of slow motions.

6. Evaluate eigenvectors $v_1, v_2, ..., v_{n_f}$ corresponding to big eigenvalues and eigenvectors $w_1, w_2, ..., w_{n_s}$ corresponding to small eigenvalues. Vectors $v_1, v_2, ..., v_{n_f}, w_1, w_2, ..., w_{n_s}$ represents a new orthogonal basis.

7. Rewrite the original system in this new coordinate system.

Let us describe a possible practical procedure for an evaluation of the matrix $T$. Fix a point $Z$ in the phase space. In many practical cases, it can be a point that represents initial data or a singular (equilibrium) point or another special point that depends on a nature of a considered problem. Then construct the linear transformation $T$ that maps a linearly independent set of vectors $Z + \Delta v_i; i = 1, 2, ..., n$ into the vectors $\Theta(Z + \Delta v_i)$.

The matrix of this linear transformation can be easily evaluated in the original coordinate system. Accordingly, if we use the notations: $F = \{Z + \Delta v_1, ..., Z + \Delta v_n\}$ and $E = \{e_1, e_2, ..., e_n\}$ for the basis of original coordinate system, then the transformation matrix is given by

$$[T(Z)]_E^F = [T(Z)]_E^F [I(Z)]_F^E = [T(Z)]_E^F \left([I(Z)]_F^E\right)^{-1}$$
Here the matrix \( [I(Z)]_E^F \) transforms the standard basis \( e_1, e_2, ..., e_n \) into the basis

\[
Z + \Delta v_1, Z + \Delta v_2, ..., Z + \Delta v_n
\]

and \( [T(Z)]_E^F \) transforms, in turn, this basis into the basis of eigenvectors. Therefore, the matrix \( [T(Z)]_E^F \left( [I(Z)]_E^F \right)^{-1} \) transform the standard basis into the basis of eigenvectors of the matrix \( T \cdot T^* \).

It is obvious that this transformation strictly depends on the chosen vectors of initial (not original) basis \( F \) and on the approximation parameter \( \Delta \).

This means that we can use different basis vectors in \( F \) as well as take the parameter \( \Delta \) changing or having a vector form, but assuming that the system has a very large gap between the different scales the influence of this choice should be in high orders of magnitude.

6.2. GQL - application

To illustrate both the idea and application of the suggested method of global quasi-linearization (TILDM and QILDM or GQL), let us consider an example describing enzyme interaction inside a biological cell, the so called Michaels-Menten model [23]:

\[
\begin{align*}
\frac{dx}{dt} &= -xz - L_1(1 - z - \mu(1 - y)), \\
\frac{dy}{dt} &= -L_3yz - \frac{L_2}{L_4}(1 - y), \\
\frac{dz}{dt} &= \frac{1}{L_2}((-xz + 1 - z - \mu(1 - y) + \mu(-L_3yz - \frac{L_2}{L_4}(1 - y)) \tag{49}
\end{align*}
\]

It is obvious that in this model studied by many authors [33, 34] the internal asymptotic structure can be found analytically but our purpose to use this example as test for the fast manifold construction. As one can easily see (Figure 7) for this set of the system parameters the system (47) - (49) has three sufficiently different time scales. First, when the system trajectory is relaxed on the two dimensional slow surface and then inside this “slow” manifold it distinguishes additional separation into fast and slow and the trajectory finally approaches the one dimensional slow manifold.

Next Figure 8 presents two dimensional structures (fast and slow manifolds) based on the TILDM with constant matrix based on initial points \( Z_{in}^{(1)} \) and \( Z_{in}^{(2)} \).

Two dimensional manifolds for both fast and slow parts are used here only for an illustration purposes because if we take a formally determined dimension of the fast manifold be two then we will have the slow manifold of only dimension one(determined by the co-dimension).

Figure 8(a) shows, in particular, that the method based on a Jacobian cannot be applied for global exploration of the fast/slow decomposition and for the approximation of the fast manifold. Last figure 8(b) represents both fast and slow manifolds, both have dimension two. These two surfaces represent rather good approximations for the fast surface and slow surface correspondingly as well as for the projection point \( Q \) (intersection of the fast manifold with slow one if we take the dimension of the slow to be one - see Figures 7 and 8). This means that if we are interested in one dimensional system dynamics we can use the fast/slow decomposition for finding the one dimensional manifold and projecting the initial point into this curve. Additionally, the quasi-linearization procedure in this very simplified form produces a fast/slow decomposition on the basis of one initial point.
Figure 7. (a) One dimensional slow system manifold $AB$, two system trajectories starting at the points $Z^{(1)}_m = (2, 0, 1)$ and $Z^{(2)}_m = (1.5, 0, 1)$. (b) One ($AB$) and two dimensional ($2$) slow manifolds produced by TILDM method (System parameters are taken as $L_1 = 0.99$, $L_2 = 1$, $L_3 = 0.05$, $L_4 = 0.1$, $\mu = 0.99$)

Figure 8. (a) Two dimensional fast/slow surfaces produced by TILDM algorithm, the matrix $Q$ is taken constant at at initial point. (b) Two dimensional fast/slow system manifolds with the system trajectory by applying GQL technique with constant matrix calculated at initial point $T(Z_m)$, $\delta = 0.1$ and $v_1, ..., v_n$ is taken as standard basis. (The system parameters are the same as in the Figure 7)

These very preliminary results show that the proposed technique, which conditionally called global quasi-linearization (GQL) might be rather helpful for a numerical analysis of systems with "hidden" hierarchical structure. The presence of the hierarchy presumes the existence of sufficiently different time scales of the processes involved. This situation is typical for combustion theory, chemical kinetics, biology and other fields of science.
7. Conclusions

Summarize main results of the present work devoted to a decomposition of systems (ODEs or PDEs). The problem is under detailed investigation by a large number of researchers during the last decades and there are large number of papers devoted to the problem (very small part of them, of direct relevance of the present manuscript, are cited here). The authors suggest their own point of view to the decomposition problem and propose a number of algorithms, which allow one to perform the decomposition for various types of systems.

The authors’ point of view is based on the assumption that the main goal of existing techniques is a construction of a new coordinate system, in which an original system can be represented as an SPS of ODEs. Most of these decomposition procedures can be interpreted as realizations of this general theoretical algorithm, which are mainly focused on the localization of the slow (attractive) invariant manifolds. The main part of these algorithms use Jacoby matrix for identification of the fast and slow motions (the fast and the slow subsystem of an original system). We demonstrate (on simple linear models) that the Jacoby matrix is not appropriate for the decomposition in a general case and that can contain relevant information only in a vicinity of slow invariant manifolds.

The authors suggest a new point of view on the decomposition issue and propose a number of algorithms, which allow identification of fast and slow motions. These algorithms are based on a new concept of singularly perturbed vector fields and permit one to perform the decomposition for various types of highly nonlinear ODE systems. The authors’ point of view is based on the idea that one should consider separately local and global decomposition approaches. Both approaches have their own advantages and disadvantages. As a result the present manuscript generally involves two approaches, devoted to the problem of local and global decompositions, correspondingly. In turn, the local approach is subdivided into different techniques, which are able to approximate separately fast and slow subsystems of the original system of ODEs. The present paper contains a description (with relevant examples) of the numerical tool (TILDM) allowing us to uncover the slow manifolds and an algorithm for approximation of the fast part of the system trajectory (dynamic decomposition approach).

The TILDM technique is a modification of well established ILDM technique and was proposed by the authors in collaboration with Prof. Ulrich Maas. It represents a result of the comparative analysis of the two powerful asymptotic methods - ILDM and MIM. The complementary properties of these two asymptotic approaches leads to an idea about existence of a feasible combination of these methods. Theoretically, this combination should be able to combine the advantages of these two approaches and to avoid their weaknesses.

ILDM was originally constructed to numerically handle systems of ODEs containing a large number of equations. As every other algorithm, ILDM has its own restrictions, which were partially demonstrated in the present paper on some elementary examples. It was shown, that ILDM can not treat regions in the phase space, where eigenvalues of a Jacobian are complex with equal real parts. Therefore ILDM can not indicate any splitting, whereas the original system can have a fast/slow subdivision. To overcome this problem a modification (TILDM) of the ILDM method was suggested.

The suggested algorithm successfully works with systems having an internal hierarchy in the regions of the complex Jacobian’s eigenvalues with close real parts because of the simple fact that the new approximating matrix is symmetric with no complex eigenvalues. It is shown that the suggested TILDM technique also has no difficulties in so-called transition zones (turning manifolds) between different branches of slow manifolds (stable and unstable), which cannot be correctly described by the ILDM method. For these zones a division into ”large” and ”small” eigenvalues of the Jacobian typically does not exist. The reason is that TILDM produces an approximation of the whole invariant manifold and not only its stable part.

It is also concluded that the TILDM algorithm is more sensitive to the ”hidden” hierarchy of
the original system than ILDM. As was also mentioned, the TILDM technique aims to determine a location of the slow manifolds, the problem, which is commonly of use in combustion problems. Nevertheless, the problem of identifying the fast part of the trajectory of an arbitrary system of ODEs is of no less importance.

To deal with fast manifolds, a new method of numerical solution of multiscale systems of ODEs is suggested (developed in collaboration with Prof. Sergei Sazhin and Dr. Elena Sazhina). The method is based on a decomposition technique for the considered system of ODEs using the same geometrical version of MIM. The comparative analysis of the values of the right hand sides of these equations, can result in the separation of the variables into fast and slow ones. The hierarchy of the decomposition is allowed to vary with time. Hence, this type of a decomposition can be called dynamic decomposition. Equations for fast variables are solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. This is considered as a zeroth order solution for these variables. The solution of equations for slow variables is presented in a simplified form, assuming linearised variations of these variables during the time evolution of the fast variables. This is considered as the first order approximation for the solution for these variables or the first approximation for the fast manifold. This approach is applied to the analysis of the problem of explosion of a polydisperse spray of diesel fuel for the parameters typical for the vicinity of the nozzle and the periphery of the spray. Our results show clear advantages of the new approach from the point of view of accuracy and CPU efficiency compared with the conventional approach widely used in CFD codes. The latter is called the fixed decomposition approach. The difference in the solutions of dynamically decomposed and full systems of equations is shown to be negligibly small for practical applications.

All the methods mentioned above have a local nature either by construction restrictions as in fast motion integration in CFD modeling or by sheme of slow dynamics only (ILDM-like techniques) and can not be useful in reducing the system dimension in a global sense. Thus, these methods are not able to decompose and describe correctly both fast and slow system dynamics simultaneously. To overcome this difficulty a novel approach to build a global transformation is proposed. The transformation aims to be valid within some bounded domain and should allow to transform the original system of ODEs into conventional SPS form.

The global character of the proposed transformation is the principal distinction of this approach from the other techniques suggested. The transformation is based on so-called the global quasi-linearization (GQL) of a vector field. It is important to note that on one hand global character is the advantage of the proposed method because of the possibility to describe both fast and slow dynamics simultaneously, and from another hand one should take high order approximations to ensure better accuracy of the reduced dynamics. Moreover, quasi-linearization can be useful for special parametric domains and comparatively simple vector fields. Fortunately, a lot of practical situations of real practical interest exist, where these approximations are applicable. The preliminary results show that the proposed technique might be rather helpful in the numerical analysis of the systems with "hidden" hierarchical structure (typical for combustion theory, chemical kinetics, biology and other fields of science).

Finally, we note that although the proposed algorithms do provide a more accurate dynamical picture than existing ones, they are not without their own deficiencies. In particular, the authors would like to underline, that at the current stage of the development, they represent mostly empiric algorithms, which have not a convincing proof or rigorous justification (in pure mathematics meaning). Looking for a rigorous mathematical justification looks as one of the possible directions of the further research. It is undisputable that a more thorough theoretical study of the suggested approach should be performed as well as scrutinized applications to other real world problems. This direction of further improvement of suggested approach is currently under investigation.
Acknowledgments
The authors are grateful to the German-Israeli Foundation (Grant G-695-15.10/2001) for the financial support of the performed work. VB gratefully acknowledges the Minerva Fellowships Program for its support.

References
[1] Babushok V I and Gol’dshtein V M 1988 Structure of the Thermal Explosion Limit Combustion and Flame 72 221
[2] Bogolyubov N N and Mitropolsky Yu A 1961 Asymptotic Methods in the Theory of Nonlinear Oscillations (New York: Gordon and Breach)
[3] Bykov V, Goldfarb I, Gol’dshtein V and Greenberg J B 2002 Thermal explosion in a hot gas mixture with fuel droplets: a two reactants model Combustion Theory and Modelling 6 1-21
[4] Bykov V, Goldfarb I, Gol’dshtein V and Maas U 2004 IMA journal of Applied Mathematics submitted
[5] Bykov V, Goldfarb I and Gol’dshtein V 2005 Multi-Scale Analysis of Pressure Driven Flames Singular Perturbations and Hysteresis, Edited by Michael P. Mortell, Robert E. O’Malley, Alezei Pokrovskii, and Vladimir Sobolev Chapter 9
[6] Davis M and Skodje R Geometric Investigation of Low-Dimensional Manifolds in Systems Approaching Equilibrium Journal of Chemical Physics 111(3) 859
[7] Fenichel M 1979 Geometric singular perturbation theory for ordinary differential equations J. Differential Equations 31 53
[8] Frank-Kamenetskii D A 1969 Diffusion and Heat Exchange in Chemical Kinetics 2nd ed. (New York: Plenum Press)
[9] Gear C, Kaper T, Kevrekidis I and Zagaris A 2005 Projecting to a slow manifold: singularly perturbed systems and legacy codes SIAM Journal of Dynamical Systems A 251 394
[10] Goldfarb I, Gol’dshtein V and Kuzmenko G 1999 Pressure Driven Flame in Porous Media Physics Letters A 251 394
[11] Goldfarb I, Gol’dshtein V and Zinoviev A 2001 Delayed thermal explosion in inert porous matrix filled with evaporating liquid fuel Proceedings of the 18th Int. Coll. on the Dynamics of Explosions and Reactive Systems
[12] Goldfarb I, Gol’dshtein V and Zinoviev A 2002 Delayed Thermal Explosion in Porous Media: Method of Integral Manifolds IMA journal of Applied Mathematics 67 263
[13] Goldfarb I, Gol’dshtein V, Katz D and Sazhin S S Radiation effect on thermal explosion in a gas containing evaporating fuel droplets, latest stages of preparation
[14] Goldfarb I, Gol’dshtein V, Kuzmenko G and Greenberg J B 1998 On Thermal Explosion of a Cool Spray in a Hot Gas Proceedings of the Combustion Institute Pittsburgh 27 2367
[15] Goldfarb I, Gol’dshtein V, Kuzmenko G and Sazhin S S 1999 Thermal radiation effect on thermal explosion in gas containing fuel droplets Combustion Theory and Modelling 3 769
[16] Goldfarb I, Gol’dshtein V and Maas U 2004 Comparative analysis of two asymptotic approaches based on integral manifolds IMA journal of Applied Mathematics 69 353
[17] Gol’dshtein V and Sobolev V 1988 Qualitative Analysis of Singularly Perturbed Systems (Novosibirsk: Institute of Mathematics Siberian Branch of USSR Academy of Science in Russian)
[18] Gol’dshtein V and Sobolev V 1992 Integral manifolds in chemical kinetics and combustion Singularity theory and some problems of functional analysis American Mathematical Society 73
[19] Gol’dshtein V, Zinoviev A, Sobolev V and Shchepakina E 1996 Criterion for Thermal Explosion with Reactant Consumption in a Dusty Gas Proc.R.Soc.Lond. A 452 2103
[20] Hadjinicolaou M and Goussis D M 1999 Asymptotic Solutions of Stiff PDEs with the CSP Method: the Reaction Diffusion Equation SIAM journal of Scientific Computing 20 781
[21] Hale J 1969 Ordinary Differential Equations (New york: Wiley)
[22] Kaper H G and Kaper T J 2001 Asymptotic Analysis of Two Reduction Methods for Systems of Chemical Reactions Argonne National Lab preprint ANL/MCS-P912-1001
[23] Laidler K J and Bunting P S 1973 The Chemical Kinetics of Enzyme Action 2nd Edit. (Oxford: Clarendon)
[24] Lam S H and Goussis D M 1988 Understanding Complex Chemical Kinetics with Computational Singular Perturbation Proc. Comb. Inst. 22 931
[25] Lam S H and Goussis D M 1994 The GSP method for simplifying kinetics International Journal of Chemical Kinetics 26 461
[26] Maas U 1994 Automatische Reduktion von Reaktions mechanismen zur Zimulation reaktiver smomungen Hasilitation Thesis (Stuttgart: Universitat Stuttgart)
[27] Maas U and Pope S B 1992 Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space Combustion and Flame 117 99
[28] Masias A, Diamantis D, Mastorakos E and Goussis D M 1999 An algorithm for the construction of global reduced mechanisms with CSP data Combustion and Flame 117 685
[29] Mitropolskiy Yu A and Lykova O B 1968 Lectures on the methods of integral manifolds (Kiev: Institute of Mathematics Ukrainen Akademy of Science in Russian)
[30] McIntosh A C, Gol'dshtein V, Goldfarb I and Zinoviev A 1998 Thermal explosion in a combustible gas containing fuel droplets Combustion Theory and Modelling 2 153
[31] Neophytou M K, Goussis D M, Van Loon M and Mastorakos E 2004 Reduced chemical mechanism for atmospheric pollution using Computational Singular Perturbation analysis Atmospheric Environment 38 3661
[32] Rhodes C, Morari M and Wiggins S 1999 Identification of the Low Order Manifolds: Validating the Algorithm of Maas and Pope Chaos 9(1) 108
[33] Roussel M R 1997 Forced-convergence iterative schemes for the approximation of invariant manifolds Journal of Mathematical Chemistry 21 385
[34] Roussel M R and Fraser S J 2001 Invariant Manifold Methods for Methabolic Model Reduction Chaos 11(1) 196
[35] Sazhin S S, Feng G, Heikal M R, Goldfarb I, Goldshtein V and Kuzmenko G 2001 Thermal ignition analysis of a monodisperse spray with radiation Combustion and Flame 124 684
[36] Sazhin S S, Sazhina E M, Heikal M R, Maroney C and Mikhalovsky S V 1999 The Shell autoignition model: a new mathematical formulation Combustion and Flame 117 529
[37] Semenov N N 1928 Zur Theorie des Verbrennungprozesses. Z. Phys. Chem. 48 571
[38] Strygin B B and Sobolev V A 1988 Decomposition of motions by the integral manifolds method (Moscow: Nauka, in Russian)
[39] Valorani M and Goussis D M 2001 Explicit Time-Scale Splitting Algorithm for Stiff Problems: Auto-Ignition of Gaseous Mixtures behind a Steady Shock Journal of Computational Physics 169 44
[40] Westbrook C K and Dryer F L 1981 Simplified reaction mechanism for the oxidation of hydrocarbon fuels in flames Combustion Science and Technology 27 31