On transformation to the singularly perturbed system

Journal of Physics: Conference Series **268** (2011) 012003 doi:10.1088/1742-6596/268/1/012003

On transformation to the singularly perturbed system

V Bykov

Institute of Technical Thermodynamics
Karlsruhe Institute of Technology (KIT)
Engelbert-Arndold-Strasse 4, Geb. 10.91
D-76131 Karlsruhe, Germany

E-mail: viatcheslav.bykov@kit.edu

Abstract. A rapid progress in hard- and software development of computational facilities as well as in numerical methods has increased the role of numerical simulations in the quantitative system analysis of many engineering problems. At the same time, the system complexity (in terms of dimensionality and non-linearity) has grown considerably increasing demand for automatic methods of analysis of qualitative system behavior. For instance, nowadays, definition of key system parameters controlling the system dynamics and finding critical regimes automatically have become crucial issue of numerical system analysis. In the present paper a transformation to the Singularly Perturbed System (SPS) as a main theoretical framework to cope with the complexity and high dimensionality will be discussed in detail. Both simple but famous and meaningful model example of Van der Pol oscillator and an example of application to numerical analysis of chemical kinetics mechanisms will be used to show the potential of the suggested framework.

1. Introduction

Power of modern computational facilities increases rapidly over last decades, more and more detailed physical and mathematical models of various phenomena become treatable by numerical system analysis via numerical simulations. Numerical experiments are considered as a powerful tool of modern research taking a leading role in science, engineering and industry. In the last decade, for instance, if one has a look at chemical kinetics (see e.g. [1] in combustion, [2, 3] - atmospheric chemistry and [4, 5] in biochemistry etc.) one realizes that the dimension of the considered system of governing equations increases almost uncontrollable.

However, the increase of the system dimension and complexity might lead to loss of reliability of the results. Understanding and interpretation of results of simulations of such systems becomes problematic. It is not easy to elucidate key system parameters and their combinations governing distinguished dynamical regimes.

In many cases, however, it is quite often one does not need such complicated description of the phenomenon under consideration, most likely the detailed model has been developed to cover and to 'fit' all possible ranges of observations and experimental data whose amount constantly grows up with time. But, in particular simulations, only a small part a certain 'sub-model' can be efficiently used to reach required accuracy and level of prediction.

Thus, one has the detailed model, from one hand side, which reflects the current situation of the detailed model development for the whole range of observations, but from the other hand in numerical treatments/simulations only a 'small part' of this model is actually involved and important, while the rest is not relevant and redundant. In order to formalize this observation and develop a tool of automatic model reduction, i.e. the tool of automatic identification of such sub-model, the coordinate free singular perturbation approach has been developed [6, 7] last few years.

The basic idea behind the approach is in using low dimensional invariant (integral) manifolds embedded into the detailed system phase space, which reflect appropriate asymptotic limits for particular application of the detailed model for numerical simulation and analysis of system dynamics. In other words, the phase space of the detailed system is assumed to be split asymptotically into family of fast/slow invariant manifolds representing relatively slow and fast system motions.

This means the decomposition of motions becomes the main assumption of our approach. It is justified by the fact that in particular situations not all phase or state space of the original detailed system are accessed by the system solution trajectories. In a wide range of system's initial, boundary conditions as well as for a wide range of system parameters the system solution is often restricted to a subset, which is in many applications can be approximated by low-dimensional invariant manifolds (see e.g. [8, 9] for more details, where the decomposition is handled implicitly). Following this assumption one concludes that if there is a simplified (in terms of dimension) or reduced model satisfactory describing the detailed one, then it should correspond to the invariant manifold of low dimension. While the overall system dynamics can be restricted to this manifold.

Accordingly, the problem of model reduction or the problem of adequate modeling reduces to identification such manifolds in the system's phase space and study these properties. One is interested in an approach which for a given detailed model (system of governing equations, range of initial, boundary and system parameters are supposed to be known) performs

- decomposition of motions;
- singular versus regular perturbation analysis;
- definition appropriate manifolds for reduced model formulation;
- restriction or projection the overall system to these manifolds.

In the present paper, the transformation to the standard form of singularly perturbed system (SPS) by using singularly perturbed vector fields approach is represented and discussed as an ideal candidate for a theoretical framework that can be very efficient for model reduction. It is illustrated on both analytical and numerical levels by well known model of Van der Pol oscillator and by application to an auto-ignition problem of combustion theory.

2. SPVF: analytical approach, Van der Pol oscillator

The main and the key idea of the suggested approach is to find a transformation to the standard SPS system form, which allows straightforward application of powerful and well developed methods of perturbation analysis. Accordingly, a number of interesting questions arise, which are in the focus of the current study. Namely,

(i) Suppose one has such a system, which is overdetermined in the sense that more parameters and equations are used than needed for adequate description of particular phenomenon under investigation. How to check this? If the answer on the previous question is positive, then

(ii) How to estimate appropriate dimensions?

(iii) How to transform the system to the explicit decomposed form as the SPS system?

2.1. Van Der Pol oscillator, original model

In order to illustrate very important technical part of the suggested method and to address motivation of the paper, let us consider the well known system of Van der Pol oscillator in its original form given by

$$\ddot{x} - \mu\left(1 - x^2\right)\dot{x} + x = 0, \tag{1}$$

written in the phase coordinates (x, y), $y = \dot{x}$ as shown in figure 1 (left), equation (1) becomes equivalent to

$$\begin{array}{c} \frac{dx}{dt} = y \\ \frac{dy}{dt} = -x + \mu\left(1 - x^2\right) y \end{array} \tag{2}$$

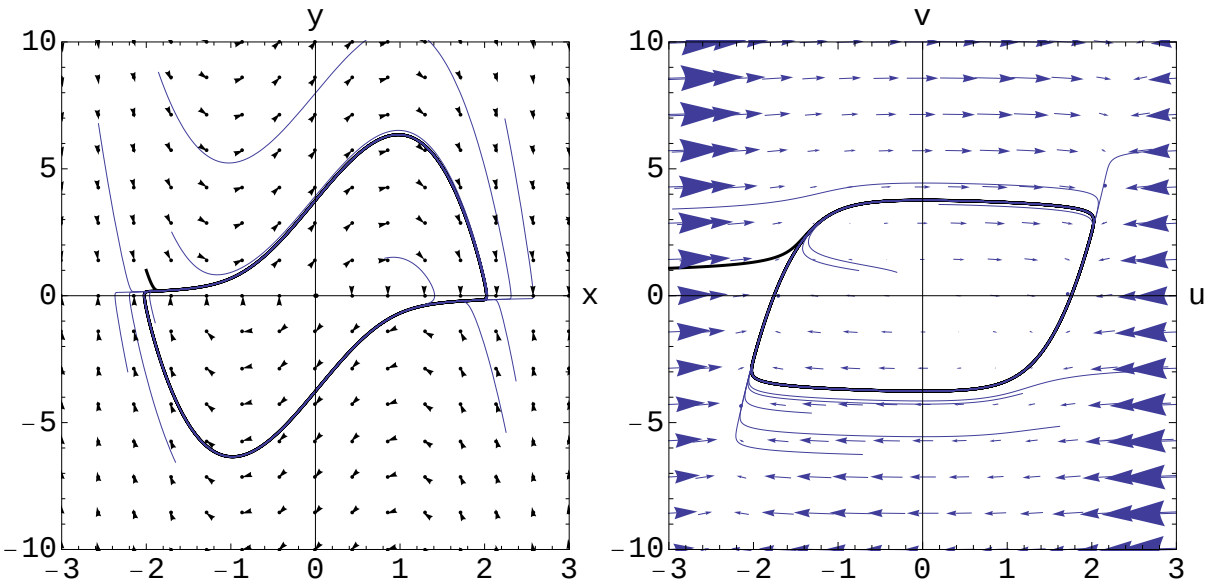

Figure 1. Phase space of the Van der Pol oscillator in the original coordinates (2) (left) and in the Lienard's coordinates (5) (right) with particular solutions trajectories and vector field.

This is an example of well known Lienard's system [10]

$$\ddot{x} + f\left(x\right)\dot{x} + g\left(x\right) = 0. \tag{3}$$

It can be considered as a well known example of one of the first successful transformation to the SPS standard form, i.e. in his study of (4) Lienard has suggested to transform the system coordinates in (4) according to

$$\begin{array}{c} u = x \\ v = \int f\left(x\right) dx + \dot{x} \end{array}\ , \tag{4}$$

which to be applied to (4) allowed to obtain well known simpler model of non-linear oscillations in the phase space coordinates, which is typically referenced as the Van der Pol oscillator (see figure 1 right)

$$\begin{array}{c} \frac{du}{dt} = v + \mu\left(1 - \frac{1}{3}u^2\right) u \\ \frac{dv}{dt} = -u \end{array}\ . \tag{5}$$

However, while looking at phase spaces of both systems one immediately realizes the difference between the models (just compare phase portraits shown in figure 1). The second representation in the Lienard's coordinates is more preferable, one can easily see two stages of the oscillatory behavior because the system is represented in the decomposed form, e.g. the first equation represents the fast system motions, while the second governs the slow system evolution. The transformation 4 decomposes of motions of Van der Pol model.

2.2. Van der Pol model with known decomposition

The main question of this subsection is the following: 'Is there a rigorous way to proceed and find transformation (4) and reconcile the meaning of the transformation?'. In order to answer this question and illustrate powerful technical skills of the suggested method let us rescale $\varepsilon\, d\tau = dt$ the time in (3)

$$\frac{d^2x}{d\tau^2} + \varepsilon\, f\,(x)\,\frac{dx}{d\tau} + \varepsilon^2 g\,(x) = 0. \tag{6}$$

Hence, in the phase space the original model of Van der Pol model becomes

$$\begin{array}{c} \frac{dx}{d\tau} = y \\ \frac{dy}{d\tau} = -\varepsilon^2 x + \varepsilon\mu\,(1-x^2)\,y \end{array}. \tag{7}$$

Now, we apply the suggested SPVF similar to [6]. The proposed framework allows to redefine the global transformation on the basis of knowledge about multiple time scales $\varepsilon\mu \sim O\,(1)$ explicitly present in the scalled form (6). According to [6], initial step is a decomposition of the vector field

$$F = F_f + F_s, \tag{8}$$

where fast - F_f and slow - F_s sub-fields of the original vector field (6) are easily found due to the explicit small parameter ε as

$$\begin{array}{c} F_f = \left(\begin{array}{c} F_{f,1} \\ F_{f,2} \end{array}\right) = \left(\begin{array}{c} y \\ \varepsilon\mu\,(1-x^2)\,y \end{array}\right), \\ F_s = \left(\begin{array}{c} F_{s,1} \\ F_{s,2} \end{array}\right) = \left(\begin{array}{c} 0 \\ -\varepsilon^2 x \end{array}\right). \end{array} \tag{9}$$

In order to represent the system as a SPS system one can proceed with the analysis of these sub-fields separately. This will lead to considerable simplification which is very important in an analytical study because it can reduce the system dimension and allows to work with much simple subsystems. For instance, if full system is considered, it is not a simple task to find the solution in any form, while the fast sub-field (subsystem) with $z = (x, y)$

$$\frac{dz}{d\tau} = F_f(z), \tag{10}$$

can be integrated easily and has the general solution in an implicit form given by

$$v = y - \varepsilon\mu\left(1 - \frac{1}{3}x^2\right)x + C_v = 0, \tag{11}$$

which means the fast motion is realized in the (x, y) plane on cubic parabola - $y - \varepsilon\mu\left(1 - \frac{1}{3}x^2\right)x + C_v = 0$ (see figure 2, left; where fast manifolds $\varepsilon = 1$, $\mu = 4$, $C_v = 0, \pm 2, \pm 4, \pm 6$ are shown by solid lines), this defines a family of fast manifolds - $\{M_{(x,y)}\}$. Moreover, the new variable v defined in this way, governs the slow system dynamics of the original system while

$$\frac{dv}{d\tau} = v_x \frac{dx}{d\tau} + v_y \frac{dy}{d\tau} = v_x \left(F_{f,1} + F_{s,1}\right) + v_y \left(F_{f,2} + F_{s,2}\right) = v_x F_{s,1} + v_y F_{s,2} \sim O(\varepsilon^2).$$

At the same time the slow subsystem

$$\frac{dz}{d\tau} = F_s(z),$$

obeys simple integral

$$u = x + C_u = 0, \tag{12}$$

and it is expected to represent fast motion (just compare to the previous system) according to

$$\frac{du}{d\tau} = u_x \frac{dx}{d\tau} + u_y \frac{dy}{d\tau} = u_x \left(F_{f,1} + F_{s,1}\right) + u_y \left(F_{f,2} + F_{s,2}\right) = u_x F_{f,1} + u_y F_{f,2} \sim O(1).$$

Hence, the standard SPS form of the system is redefined by using (11-12) as

$$\frac{du}{d\tau} = u_x F_{f,1} + u_y F_{f,2} = F_{f,1}\left(u, v\right) = v + \varepsilon\mu \left(1 - \frac{1}{3}u^2\right) u,$$

$$\frac{dv}{d\tau} = v_x F_{s,1} + v_y F_{s,2} = F_{s,2}\left(u, v\right) = -\varepsilon^2 u.$$

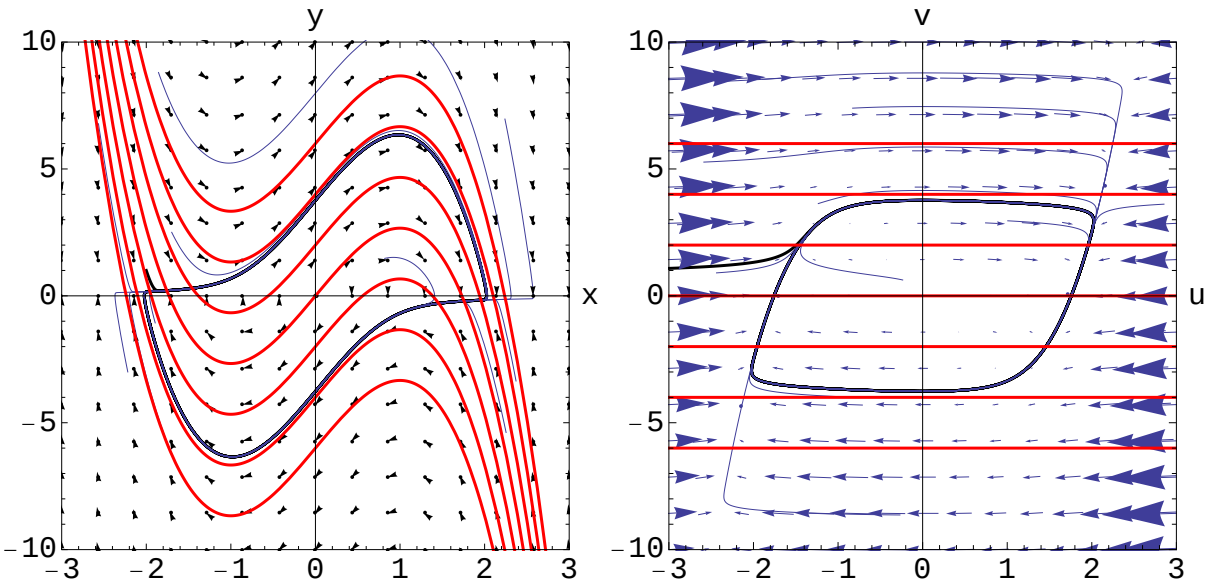

Figure 2. Phase space of the Van der Pol oscillator with fast manifolds (11) (red) as defined by the SPVF analysis in the original coordinates (2) (left) and in the Lienard's coordinates (5) (right) with particular solutions trajectories and vector field.

Here constants - C_u, C_v were chosen to be equal to zero in the coordinate change. Moreover, when the scaling factor is set to be one, the system purely coincides with the Lienard form of the original Van der Pol model. It means that the suggested procedure to check the system hierarchy and decompose the system fully reconciles the Lienard's change of the system variables to simplify the Van der Pol system representation.

3. SPVF: numerical approach, auto-ignition problem

In the previous section it was shown how the SPVF theory can be analytically applied if the decomposition is known explicitly. However, more interesting and complicated question concerns situations where there is no additional internal information available. Although our approach is very general, by now main applications are in reacting flow modelling.

3.1. Invariant manifolds method and connection to the decomposition

Consider a very simple model describing chemically reacting system, which is a pure homogeneous system. It is represented by a system of ordinary differential equations (ODEs) that describes the chemical kinetics mechanism by the system based on the mass action law. The equations of the system describe the evolution of the thermo-chemical state vector

$$\Psi = \left(h,\, p,\, \frac{w_1}{M_1}, ...,\, \frac{w_{n_s}}{M_{n_s}}\right)^T, \tag{13}$$

in time, where Ψ_i represents such quantities as the pressure of the mixture p, the enthalpy h, i.e. two thermodynamic quantities and specific mole numbers w_i/M_i (the mass fractions w_i divided by molar mass M_i) or mole fractions of chemical species that describe the mixture composition. In these vector notations the system of governing equations of a homogeneous system can be written in autonomous form as (see e.g. [11])

$$\frac{d\Psi}{dt} = F\left(\Psi\right), \quad \Psi \in \Omega \subset R^n. \tag{14}$$

Here the so-called chemical source term F represents the chemical kinetic mechanism comprises $A_1, ..., A_{n_s}$ chemical species ($n = n_s + 2$) participating in $i = 1, ..., n_r$ elementary chemical reactions

$$\alpha_{i,1}A_1 + ... + \alpha_{i,n_s}\, A_{n_s} \rightleftharpoons \beta_{i,1}A_1 + ... + \beta_{i,n_s}\, A_{n_s}, \tag{15}$$

The mass action low implies the polynomial form of elementary reaction rates (consider species concentrations only, i.e. $\Psi = \left(\left[A_1\right], ..., \left[A_{n_s}\right]\right)$), then the elementary reactions rates are

$$R_i\left(\Psi\right) = k_i^+ \prod_{j=1}^{n_s} \Psi_j^{\alpha_{i,j}} - k_i^- \prod_{j=1}^{n_s} \Psi_j^{\beta_{i,j}},\ i = 1, ..., n_r, \tag{16}$$

where $k_i^+,\ k_i^-$ are the parameters (depending on the thermodynamic properties of the system $\Psi = \left(\left[A_1\right], ..., \left[A_{n_s}\right]\right)$) of forward and inverse reactions rates typically modeled by the Arrhenius law [12]. Therefore, it yields for species evolution of $F\left(\Psi\right)$

$$F_j\left(\Psi\right) = \sum_{i=1}^{n_r} \gamma_{i,j}\, R_i\left(\Psi\right),\ j = 1, ..., n_s, \tag{17}$$

here $\gamma_{i,j} = \beta_{i,j} - \alpha_{i,j}$ components of the so-called stoichiometric vectors. Additionally, invariance of the domain Ω (composed by vectors with non-negative components) is assumed to ensure dissipative nature of chemical reaction kinetic mechanisms.

The main question 'What does it mean to reduce the system (14)?' is discussed in this subsection. One understands it as a reformulation of the system (14) in an appropriate form by introducing the so-called reduced state space $\theta = (\theta_1, ..., \theta_m),\ m \ll n$ consisting of new variables set, such that any 'particular' solution of the system (14) will be 'represented sufficiently' accurate by the reduced model

$$\frac{d\theta}{dt} = \tilde{F}(\theta), \quad \theta \in R^m. \tag{18}$$

Clearly, the question of how the detailed and reduced spaces are connected to each other has to be in the focus of any model reduction strategy. In principle, one only needs to determine how the manifold is embedded into the phase space! This, in most cases not a trivial relation, should be the subject of any reduction methodology. If the reduced space can be accurately represented in an explicit form by

$$M = \{\Psi = \Psi(\theta) : \ \theta \in R^m\}, \tag{19}$$

a low-dimensional invariant manifold M embedded in the detailed system (14) state space, then model reduction means rewriting the system (14) on M. Substitution of the relation (19) to (14) yields

$$\frac{d\Psi(\theta)}{dt} = F(\Psi(\theta)), \ \Psi_\theta \frac{d\theta}{dt} = F(\Psi(\theta)) \rightarrow \frac{d\theta}{dt} = \tilde{F}(\theta) = \Psi_\theta^+ F(\Psi(\theta)). \tag{20}$$

here Ψ_θ^+ is the Moore-Penrose pseudo-inverse [13], which is a well defined function unless the local tangent space of M given by Ψ_θ degenerates. This simple observation makes clear the importance of definition of an appropriate manifold (19) in the state space and of studies of its properties. Obviously, not any manifold is appropriate for model reduction, only those which possess properties of

(i) invariance or approximate invariance, e.g. to be exact representation of a solution of (14) or to be an approximation to the exact solution;

(ii) attractiveness, i.e. small perturbations cannot drive the solution of (14) out of the manifold (19));

(iii) existence in the whole domain of interest, i.e. it has to approximate the detailed system (14) solutions for sufficiently wide range of initial conditions and system parameters.

These properties will automatically guarantee the closeness of the solutions of (14) $\Psi = \Psi(t)$ and of (18) through $M : \Psi = \Psi(\theta(t))$. Therefore, there is a strong need in methods of construction of appropriate invariant manifolds in the system (14) state/phase space and in approaches that can be applied to study their properties.

3.2. GQL

Because the definition of the invariant, attractive and low dimensional manifold, and the way it is embedded into the detailed system state space, is a central point of model reduction the reduction of a given arbitrary system with prescribed dimension and accuracy is almost impossible in general. Fortunately, systems governed by chemical reactions have certain properties that, nevertheless, make the model reduction feasible.

The existence of various scales or multiple scales is the well known feature of chemically reacting flows. Both in experiments and in detailed model simulations it is observed that not the entire possible range of the thermo-chemical state space is typically accessed by the system states (solutions), but only a part of it [14]. The standard mathematical framework to handle multi-scales phenomenon is the standard SPS theory (see e.g. [15, 16] for more detail). However, it is assumed that the system is represented as the SPS in the original coordinates, which restricts considerably the applicability range of such an approach. Therefore, as pointed out above, a coordinate free approach has been developed recently [17, 18]. The main advantage of the approach is in access to the decomposition structure without being restricted to particular coordinate frame.

It is shown above by the Van der Pol model that the approach is an efficient tool of asymptotic analysis when the decomposition is known. For cases of unknown a priory decomposition structure an algorithm of Global-Quasi Linearization (GQL) for identification of the system

multi-scale hierarchy with its suitable representation has been emerged as well (see e.g. [18] for detailed description). Below a brief outline is only presented which is needed for further analysis and results presentation.

The central point of the approach is a global linear approximation or interpolation of the Right Hand Side (RHS) function of (14) given by $T\,\Psi \sim F\,(\Psi)$. It is assumed that if there are multiple scales of the reaction processes, then a gap between the eigenvalues of T can be used for decomposition. In this case two groups of eigenvalues have sufficiently different (by orders of magnitude) characteristic values. Their invariant subspaces (obtained by using the Schur decomposition and then by solving subsequently the Sylvester equation [19]) yield:

$$T = (Z_f\ Z_s) \cdot \begin{pmatrix} N_f & 0 \\ 0 & N_s \end{pmatrix} \cdot \begin{pmatrix} \tilde{Z}_f \\ \tilde{Z}_s \end{pmatrix}. \tag{21}$$

$$\tilde{Z} = Z^{-1} = (Z_f\ Z_s)^{-1} = \begin{pmatrix} \tilde{Z}_f \\ \tilde{Z}_s \end{pmatrix}, \tag{22}$$

here Z_s is the (n by m_s)-dimensional matrix belonging to the invariant subspace of the m_s eigenvalues having the smallest real parts (defined by N_s), while Z_f is the (n by m_f)-dimensional matrix related to the m_f eigenvalues (defined by N_f) having the largest real parts respectively, where m_s and m_f denotes the number of eigenvalues according to slow and fast processes. Thus, an invariant manifold describing the slow system dynamics is given as the manifold that annihilates the sub-processes spanned into the fast subspace, i.e. it defines the states where fastest processes are relaxed already

$$M_s^0 = \left\{\Psi :\ \tilde{Z}_f\,F(\Psi) = 0\right\}. \tag{23}$$

This equation system is an implicit definition of the correlation between the state variables of a reacting flow introduced by fast relaxing thermo-chemical processes. Whilst those split into slow subspace do not change during fast relaxation process, namely

$$M_f^0(\Psi_0) = \left\{\Psi :\ \tilde{Z}_s\,\Psi = \tilde{Z}_s\,\Psi_0\right\}. \tag{24}$$

Thus, new coordinates suitable for an explicit decomposition are given by

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} \tilde{Z}_f\Psi \\ \tilde{Z}_s\Psi \end{pmatrix},\ \Psi = (Z_f\ Z_s) \begin{pmatrix} U \\ V \end{pmatrix}, \tag{25}$$

where and correspond to new fast and slow variables respectively. The decomposed form

$$\begin{cases} \frac{dU}{dt} = \tilde{Z}_f F\,(\Psi(U,V)) \\ \frac{dV}{dt} = \tilde{Z}_s F\,(\Psi(U,V)) \end{cases}, \tag{26}$$

and corresponding fast and slow subsystems are

$$\begin{cases} \frac{dU}{dt} = \tilde{Z}_f F\,(\Psi(U,V)) \\ \frac{dV}{dt} = 0 \end{cases}, \begin{cases} 0 = \tilde{Z}_f F\,(\Psi(U,V)) \\ \frac{dV}{dt} = \tilde{Z}_s F\,(\Psi(U,V)) \end{cases}. \tag{27}$$

The small system parameter can be estimated by the gap between the smallest eigenvalue of the large group and the largest eigenvalue of the small group of eigenvalues [18]

$$\varepsilon = \frac{max\,|\lambda\,(N_s)|}{min\,|\lambda\,(N_f)|} \ll 1. \tag{28}$$

The reduced system dimension and the small system parameter are available due to the gap in (21) between limiting eigenvalues (28). In this way identified system's hierarchy, namely, approximations of slow, fast invariant subspaces (21), (25) and system small parameter (21) make the analysis of properties (existence, stability, invariance etc.) of the slow invariant manifold possible. For instance, the following eigenvalue problem of answers whether the points on the slow manifold (23), (24) are stable or not

$$Re\left(\lambda\left(\tilde{Z}_f\,D_\Psi F\,(\Psi^*)\;Z_f\right)\right)|_{\Psi^*\in M_s^0} < 0, \tag{29}$$

This condition means that all points of the manifold attractive to the system trajectory flow with respect to the fast manifolds. It is clear that without proper estimation of the invariant subspace of the fast motions this feature of the manifold can not be investigated. Additionally, the knowledge of the explicit decomposition (25) can be used not only to determine the slow, fast manifolds (23), (24), but it provides with possibility to improve the approximation of the slow manifold (23), for instance, an approximation of the first order of magnitude by (28) is given by

$$M_s^1 = \left\{\Psi :\; \tilde{Z}_f\,D_\Psi F\,(\Psi)\;F\,(\Psi) = 0\right\}, \tag{30}$$

where $D_\Psi F\,(\Psi)$ is the Jacobi matrix of (20). In general, the idea of the constant transformation is not new see e.g. [20], but principle point is in the developed algorithm that estimates this transformation, which produces the best decomposition with respect to existing multi-scales hierarchy.

3.3. Methane/air (C1) mechanism

In order to illustrate the analysis and main results a relatively small mechanism has been chosen [21]. It contains $n_s = 16$ species plus pressure and enthalpy, i.e. overall system dimension is 18, and $n_r = 92$ elementary reactions. By implementing the GQL at initial temperature of 1235 K (pressure 3.12 bar) one finds that there are two cases/gaps: the first gap between 8 and 9 in (21) i.e. $m_f^1 = 10$, $m_s^1 = 8$, and between 14 and 15 yielding $m_f^2 = 4$, $m_s^2 = 14$, with $\varepsilon^1 = 0.17$ and $\varepsilon^2 = 0.018$ correspondingly. Figure 3 shows the state space and profiles of the integration of these two subsystems (along with 2D GQL slow manifolds). First, the fast subsystem of 10 dimensions given by (27) in the left is implemented to represent the reduced model, and the second the slow subsystem of 14 dimensions is chosen to reduce the system (14), where 4 dimensional fast subspace is 'relaxed' (see (27) right).

Figure 4 shows the performance of two models as the fast and slow subsystem with respect to the delay times and relative errors of the reduced models. It is shown that the relative error is smaller for the slow invariant manifold approximation, which is clear because the gap condition is stronger for the slow subsystem (small parameters: $\varepsilon^1 = 0.17 \gg \varepsilon^2 = 0.018$), but both can be considered as appropriate reduced models because, typically, in applications logarithmic scales are compared for the delay times.

In particular, the performed analysis shows that the system (14) in this case can be described efficiently by the system of only 6 dimensions $n - m_s^1 - m_f^2 = 18 - 8 - 4 = 6$, because 8 linear combinations of original variables can be fixed and four processes are relaxed according to (23), (24).

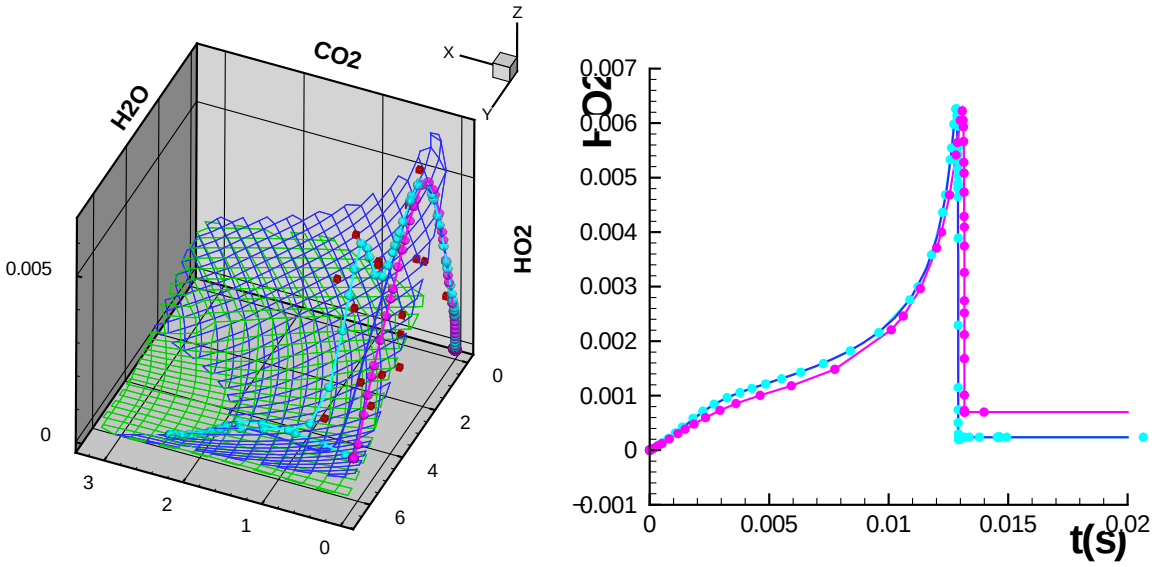

Figure 3. Results of GQL analysis of a methane/air homogeneous system shown in projection onto specific mole numbers and by solutions' profiles (right). Solid lines with symbols are fast subsystem solutions' trajectories and slow subsystem solutions, the mesh (left) is the 2D GQL slow surface. Solid line is the detailed system trajectory, cubes represent the set of point used for the GQL system analysis.

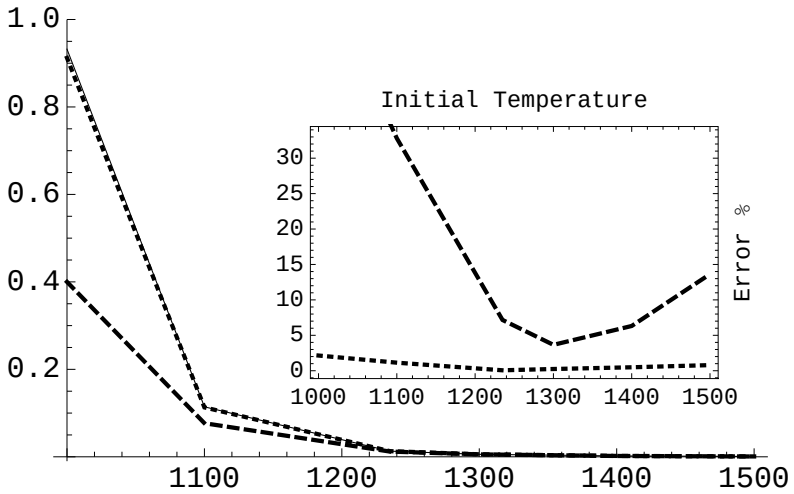

Figure 4. Delay times versus initial temperature and relative errors, the detailed model – black line, slow subsystem delay times – dotted line, fast subsystem delay times – dashed line.

3.4. Van der Pol oscillator, numerical treatment by GQL

It is interesting to compare analytical and results with numerical approach and to see what one can obtain in the case of not linear fast manifolds which, by now, is only the case when the GQL can be automatically applied. For this purpose we consider the original Van der Pol model with $\mu = 4$ and compare it with results for the transformed Van der Pol system where fast manifolds are linear (see figure 2 and 5 (right)). The results of the numerical analysis for $\Omega = [-3, 3] \times [-10, 10]$ are shown in figure 5 (left), where the red line is an approximation of the fast motion and blue line represents the slow curve. The result of the GQL analysis is

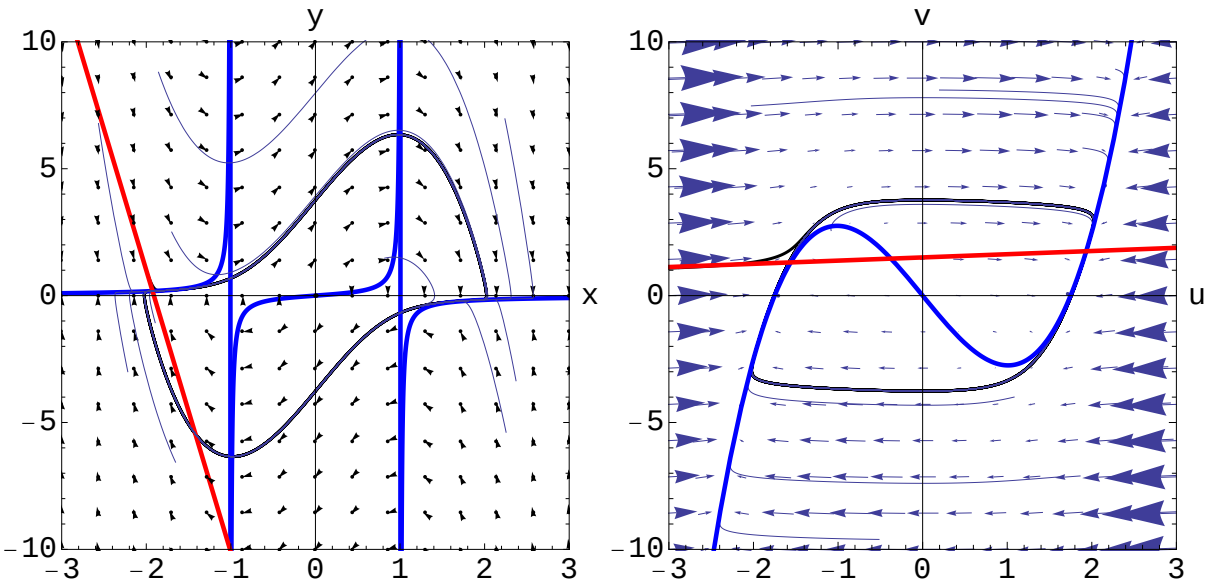

Figure 5. Phase space of the Van der Pol oscillator in the original coordinates (2) (left) and in the Lienard's coordinates (5) (right) with particular solutions trajectories and vector field. On both figures, the fast subspace of the GQL numerical analysis is shown by solid straight line (red), while the slow manifold is shown by bold solid curve (blue).

$$T = \begin{pmatrix} 0 & 1 \\ -0.96 & -8.76 \end{pmatrix}, Z = \begin{pmatrix} -0.11 & 0.99 \\ 0.99 & -0.11 \end{pmatrix}, \tag{31}$$

$$\lambda(T) = \{-8.64, -0.11\}.$$

The eigenvalues show that there is a decomposition in the considered system as it was expected (the small parameter is approximated by $\varepsilon = 0.1115$). Moreover, although the fast manifolds are not linear the slow curve, nevertheless, approximates quite well the invariant system manifold (see figure 5, where fast and slow manifolds are calculated for the Van der Pol original system (2) according to (23), (24) and (31)). Additionally, the direction of the linear fast motions, at least for a large part of the domain, given by the GQL analysis quite accurately approximate the fastest part of the non-linear fast manifolds (just compare figure 2 and 5, where fast direction represents family of non-linear fast manifolds).

4. Conclusions

In the present paper problem of model reduction and asymptotic system analysis is discussed. The problem of reduced description is represented from the invariant manifolds method point of view, which is a most suitable framework of model reduction. The natural assumption of multiple scales and the decomposition of motions allows to decouple the fast motions/processes and as a result reduce the system's dimension and stiffness. A method of coordinate free singular perturbations (SPVF) for model analysis and reduction has been discussed both at analytical and numerical levels.

The main feature of the approach in comparison to other methods is in approximating not only the slow system dynamics/manifolds, but the fast manifolds as well. Rigorous detailed analysis of system multi-scale hierarchy becomes possible. The approach can be successfully

applied in both analytical and numerical aspects to yield the explicit decomposition of the system exhibiting the multi-scale behavior. The realization and implementation of the method lead to the general scheme of an automatic reduction procedure which is based on invariant system manifolds of low dimension evaluated by the developed GQL system decomposition.

The results show that the suggested method can be efficiently implemented to define of the fast/slow invariant manifold equations, decompose system (define the explicit SPS form) and study the properties of the invariant system manifold. The method improves considerably the model reduction concept of mechanisms of chemical kinetics, it represents a rigorous approach to treat systematically kinetics mechanisms and define the decomposition of detailed model.

Acknowledgments
I would like to thank Vladimir Gol'dshtein, my former supervisor, friend and close collaborator in the developing the approach for his remarks and suggestions. Financial support from the Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged.

References
[1] Warnatz J, Maas M, Dibble R W 2004 *Combustion* 4 edn. (Springer-Verlag, Berlin Heidelberg)
[2] http://jpldataeval.jpl.nasa.gov/
[3] Atkinson et al. 2003 Summary of Evaluated Kinetic and Photochemical data for atmospheric chemistry, available at: http://www.iupac-kinetic.ch.cam.ac.uk/summary/IUPACsumm_web_latest.pdf
[4] Crampin E J, Schnell S and McSharry P E 2004 *Prog. Biophys. Mol. Biol.* **86** 177
[5] Maria G 2004 *Chem. Biochem. Eng. Q.* **18:3** 195
[6] Bykov V, Goldfarb I, Gol'dshtein V 2006 *J. Phys.: Conf. Series* **55** 28-44
[7] Bykov V, Gol'dshtein V 2008 *J. Phys.: Conf. Series* **138**, 012003
[8] Gorban A N, Karlin I V 2003 *Chem. Eng. Sci.* **58**, 4751
[9] Gorban A N, Karlin I V and Zinovyev A Yu 2004 *Physica A* **333**, 106
[10] Liénard A 1928 *Revue générale de l'électricité* **23** 901–912 and 946–954
[11] Williams F A 1985 *Combustion Theory*, 2nd ed. (Benjamin/Cummings, Menlo Park, California)
[12] Laidler K J 1997 *Chemical Kinetics*, 3rd ed. (Benjamin-Cummings)
[13] Golub G H and van Loan C F 1989 *Matrix Computation*, The Hopkins University Press (Baltimore, London)
[14] Maas U and Thévenin D 1998 *Proc. Combust. Inst.* **27** 1183–1189
[15] Fenichel N 1979 *J. Differential Equations* **31** 53–98
[16] Gol'dshtein V and Sobolev V 1992 *Amer. Math. Soc.*, Translations, ed.: S.G. Gindikin, s. 2, **153** 73–92
[17] Bykov V, Gol'dshtein V and Maas U 2008 *Combustion Theory and Modelling (CTM)* **12(2)** 389–405
[18] Bykov V and Maas U 2009 *Z. Phys. Chem.* **223(4-5)** 461–479
[19] Maas U 1993 *Habilitation Thesis*, Institut fuer Technische Verbrennung (Universitaet Stuttgart)
[20] Okino M S and Mavrovouniotis M L 1998 *Chem. Rev.* **98(2)** 391-408
[21] Smooke M D Puri I K and Seshadri K 1986 *Proc. Combust. Inst.* **21** 813–821