IMPLEMENTATION OF ILDMS BASED ON A REPRESENTATION IN GENERALIZED COORDINATES

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Abstract. *The usage of detailed chemical kinetics for the mathematical modeling of combustion processes is desirable, but leads to a high computational effort. In the present work one of the methods of simplification of chemical kinetics - Intrinsic low-dimensional manifolds (ILDMs) is considered. Whereas in most CFD applications ILDMs are calculated in terms of a fixed parameterization given by, e.g., concentrations of major species, a locally adapted parameterization procedure is introduced in terms of so-called generalized coordinates. The problem of non-existence of ILDMs in parts of the domain of interest of the state space is overcome by an extension procedure based on simplified stationary solutions. These modifications improve numerical stability, performance and guarantee uniqueness of tabulated manifolds. Sample calculations of laminar flames verify the approach.*

1 INTRODUCTION

The simulation of reacting flows using detailed chemistry introduces a large number of species (sometimes it may reach more than 1000) and reactions. This leads to a large number of species conservation equations and to a time consuming evaluation of the chemical source terms. Furthermore, the non-linearity of the the chemical source terms leads to a high stiffness of the governing equation system. As a result, detailed chemical kinetics are usually computationally prohibitive for modeling combustion flows and it is necessary to devise methods to reduce chemical kinetics[1]. The concept of ILDM (Intrinsic Low Dimensional Manifolds)[2, 3] is one of these techniques that has proven to be an efficient tool for an automatic simplification of chemical kinetics. Based on an eigenvalue analysis of the Jacobi matrix of the chemical source term, it generates automatically reduced mechanisms to describe the chemical kinetics by a small number of reaction progress variables without significant sacrificing accuracy.

For the successful implementation of the ILDM method two sub-tasks arise: first, an efficient generation of the reduced mechanism defined in the whole domain, and, second,

the projection of the governing equations in the CFD code to the low dimensional manifold approximating the reduced system dynamics. Concerning the first task, one point has to be underlined: in spite of many advantages of the ILDM type automatic reduction models there is principal drawback. Namely, an attractive manifold containing reduced system dynamics does not exist everywhere in the whole domain of interest in the state space. It means that the system dynamics cannot be reduced by the ILDM in some parts or in some sub-domains of the whole domain in the state space. Therefore, in such domains an alternative to the standard ILDM must be found. To overcome this a concept of domain splitting is developed and implemented in the following.

As for the projection onto the ILDM, there are several possibilities to project the governing equation system onto an ILDM. In CFD applications it is calculated in terms of a fixed parameterization. In this case, the governing equation system is projected to 2-4 major species concentrations characterizing the reaction progress (e.g. CO_2 and H_2O). This approach is intuitive, because the physical meaning of the reduced variables remains constant and is familiar. However, the use of a fixed parameterization can introduce numerical problems in zones, where the reaction progress and the ILDM are ill represented by the fixed reduced variables (i.e. the reduced variables change not significantly but the other variables do, or the representation of the ILDM is not unique). A projection of the original ILDM grid to a new grid parameterized by another set of reduced variables avoids this problem, but requires additional post-processing steps and can introduce an ill-conditioning. To avoid problems with this a calculation of the ILDM in terms of generalized coordinates is used. The ILDM is parameterized by means of a unit grid which is built up during its generation. The parameterization is locally adapted in the state space such that it follows the manifold. The use of generalized coordinates is not intuitive, because the physical meaning of the reduced variables changes and is not ostensive. The generalized coordinates are everywhere ideally adapted to the reaction progress on the reduced manifold and uniqueness is guaranteed. In particular, this corresponds to a projection of the governing equation system to local grid coordinates of the ILDM. Furthermore, due to the orthogonal structure of the grid the interpolation during the CFD calculation turns out to be robust and efficient.

The structure of the paper is the following: first a calculation of the standard ILDM in terms of generalized coordinates and the extension of the ILDM to cover all the domain of interest in the state space will be presented. After that the implementation scheme is outlined and, finally, simple calculations of 1-dimensional free and strained flames using detailed and reduced chemistry are presented and discussed.

2   EFFICIENT CALCULATION OF ILDMS

The mathematical model of the ILDM method is described in details in previous works[2]−[7]. Here, only a short repetition to outline the meaning of generalized coordinates in the context of standard ILDM shall be presented.

Typically, in chemically reacting systems (chemical reaction, flow, molecular transport)

course with time scales differing by many orders of magnitude (they vary in combustion processes from 10^{-10} to 10^0 s). This disparity in time scales leads to partial equilibria of chemical reactions and to steady states of species (i.e. fast processes are not rate limiting and correlations between species concentrations occur). By means of a separation or decomposition into fast and slow processes it is possible to decouple these fast processes and, consequently, to reduce the system dimension.

In order to present the essence of main idea, let us consider a homogeneous reaction system. The thermochemical state is completely determined by the $(n = n_s + 2)$-dimensional vector $\Psi = (h, p, \frac{w_1}{M_1} ... \frac{w_{n_s}}{M_{n_s}})^T$ where h denotes the enthalpy, p the pressure, $w_1, ..., w_{n_s}$ the species mass fractions and $M_1, ..., M_{n_s}$ the molar masses. Denote $X = (x_1, ..., x_{n_s})$ a vector of species mole fractions - $x_i = \frac{w_i}{M_i}$. The n-variables span up the n-dimensional state space [5, 8]. Accordingly, particular chemical reaction corresponds to a movement along a trajectory in this state space and is governed by the ODE equation

$$\frac{\partial \Psi}{\partial t} = F(\Psi),\tag{1}$$

here $F(\Psi)$ is the n-dimensional vector of chemical source term and t denotes the time. The $(n$ by $n)$-dimensional Jacobi matrix F_Ψ $((F_\Psi)_{ij} = \frac{\partial F_i}{\partial \Psi_j})$ of the chemical source terms is used to identify fast/slow decomposition of chemical processes by an invariant subspace decomposition of the Jacobi matrix yields

$$F_\Psi = (Z_s \ Z_f) \cdot \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \cdot \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix}.\tag{2}$$

The matrices Z, $\tilde{Z}$ span up the right invariant subspace and the left invariant subspace correspondingly,

$$\tilde{Z} = Z^{-1} = (Z_s \ Z_f)^{-1} = \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix},\tag{3}$$

here Z_s is the $(n$ by $m_s)$-dimensional and Z_f the $(n$ by $m_f)$-dimensional invariant subspace belonging to the m_s eigenvalues having the smallest real parts (N_s) and the m_f eigenvalues (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[9, 10]. The general assumption that the fast processes have already relaxed define a m_s-dimensional manifold in the state space. This subspace is composed of points where the reaction rates in direction of the n_f fast processes vanish

$$\tilde{Z}_f(\Psi)F(\Psi) = 0,\tag{4}$$

where $\tilde{Z}_f$ is the $(m_f$ by $n)$-dimensional matrix of left invariant subspace corresponding to the fast relaxing processes. Since the equation system is under-determined $m = n - m_f$

equations have to be added for the unique solution during the generation process of the ILDM (4)

$$P_z(\Psi - \Psi_p) = \alpha, \tag{5}$$

$$P_r(\Psi)(\Psi - \Psi_p) = \Delta\theta, \tag{6}$$

n_z equations parameterize the conserved quantities (element composition, enthalpy, pressure) and $n_r = m - n_z$ equations parameterize the reaction progress. α is the n_z-dimensional vector characterizing the parameters of conserved variables (in adiabatic, premixed and constant pressure systems they are kept constant and thus, α is zero), $\Delta\theta$ denotes the n_r-dimensional vector characterizing the parameters for the reaction progress. As a result, reduced mechanisms are obtained, where the thermochemical state of the system is represented by a small number of variables only, which are denoted by θ. Ψ is the demanded new point and Ψ_p is an existing point of the manifold in the neighborhood, P_z denotes the (n_z by n)-dimensional parameterization matrix which defines the mapping from the state vector to the vector of conserved variables. It is kept constant during the generation of the ILDM. By means of a further development of the solution procedure up to a multi-dimensional continuation procedure it was possible to dismiss the approach of a fixed parameterization (P_r is constant) and, instead of, to use an optimal parameterization for each point of the state space (i.e., the solution procedure adapts the parameterization in a multi-dimensional parameter space from state to state). Therefore, the (n_r by n)-dimensional parameterization matrix $P_r(\Psi)$ is adapted for each point of the manifold. Equations (4)-(6) are given locally in a neighborhood of Ψ and define a m_s-dimensional manifold in the state space where, if the state is assumed to be an element of the manifold, Ψ can be given as a function of α and θ

$$\Psi = \Psi(\alpha, \theta). \tag{7}$$

The numerical calculation is done by a path-following algorithm with predictor-corrector procedure starts on a known initial point (e.g. the equilibrium point), generates an m_s-dimensional mesh in the different coordinate directions and solves equations (4)-(6) on the nodes of the mesh cell by cell[11]. Then, the m_s-dimensional domain of the manifold is described by a mesh, which consists of m_s-dimensional hypercubes (see Fig. 1). In the following the grid indices are called generalized coordinates θ. The direction vectors of the neighboring cells

$$\Psi_{\theta_i} = \Psi_p(\theta) - \Psi_p(\theta - \delta_i), \; \delta_i = (\delta_{i1}, ..., \delta_{in_r})^T \tag{8}$$

are used to adapt the parameterization matrix $P_r(\Psi)$, where $\Psi_p(\theta)$, $\Psi_p(\theta - \delta_i)$ are cell points, δ_{ij} is Kronecker delta and $\Psi_\theta = \left(\Psi_{\theta_1}, ..., \Psi_{\theta_{n_r}}\right)$ is an approximation of the (n by n_r)-dimensional gradient of Ψ based on cell vertices with respect to θ of a neighboring cell. Insertion into equation (6) gives

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$$P_r \cdot \Psi_\theta = I, \tag{9}$$

and $P_r(\Psi)$ is defined as

$$P_r = \Psi_\theta^+, \tag{10}$$

where I is the (m_s by m_s)-dimensional unity matrix and Ψ_θ^+ the (n_r by n)-dimensional Moore-Penrose pseudo-inverse of Ψ_θ of the neighboring cell. As a result, the parameterization directions are, with a first order approximation, tangent to the manifold and, therefore, the grid coordinates ideally adapted to the ILDM where the parameterization direction corresponds to the direction of the slow eigenvectors.

The state Ψ and the invariant subspaces $Z_s(\Psi)$, $Z_f(\Psi)$ are then obtained as known functions of the m_s-dimensional vector of mesh coordinates θ

$$\Psi = \Psi(\theta). \tag{11}$$

2.1 Extension of the ILDM

It is known that the ILDM[12], especially with attractive properties, does not exist everywhere in the domain of interest of the composition space. There are several reasons for this; a major reason is the so-called low temperature domain, called "no chemistry" domain in the following where the source term is negligibly or exponentially small. In a flame this domain in the state space corresponds to the pre-heating zone.

Accordingly, the domain of interest can be separated into three different sub-domains such that in the first one the chemical kinetics governs the system dynamics, which means that the fast chemical processes always equilibrate towards some low dimensional manifold which contains the slow system dynamics and interaction of the slow sub-processes with convection diffusion ones. In the second domain the chemical and convection/diffusion processes are strongly coupled. The third one is the domain of very (infinitely) slow chemistry where the chemical source term is negligible and the system dynamics is governed by convection/diffusion only. A typical system trajectory in the state space links the equilibrium point, which always belongs to the ILDM manifold with the initial point (the initial point corresponds to a given boundary condition - unburnt point) that can be located in any of the three defined domains. Fortunately, in many practical combustion problems the second domain asymptotically shrinks into the boundary between first and third domains due to strongly non-linear (exponential) dependence of the source term on system parameters and, consequently, can be ignored or neglected without essential loss of accuracy.

The basic idea now is to overcome this problem and exploit the behavior in the different domains and to construct a matching procedure between the two domains[13]. Specifically, in the first domain the standard ILDM can be applied to obtain the reduced dynamics and
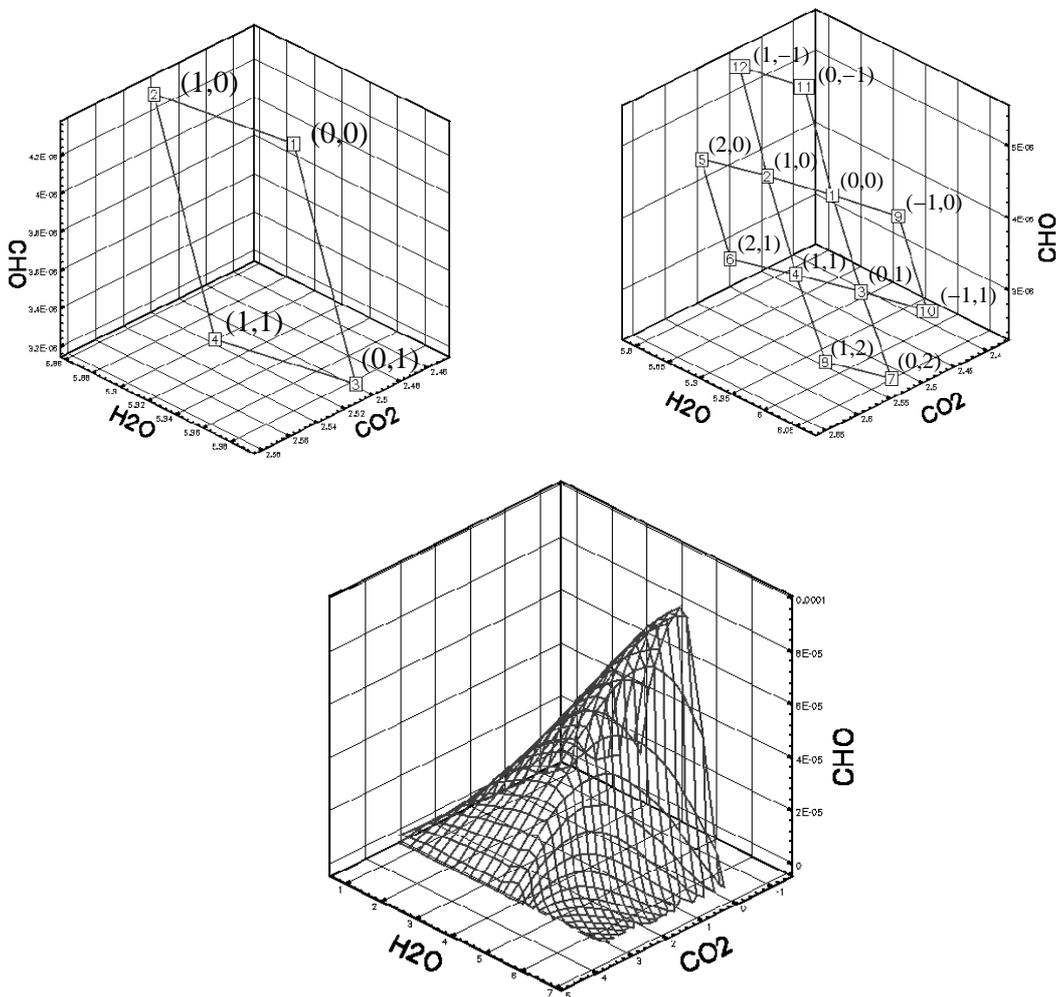
Figure 1: Stages of generation of the ILDM mesh in the state space. Vertices indices correspond to the generalized coordinates.

then extended to the third one. To understand what might be used as a suitable extension of the ILDM, consider the system (15) in the third domain with an absence of the source term and with the additional assumption of equal diffusivities. In this case the nature of the diffusion term gives rise to the fact that each linear manifold in the composition space constitutes an invariant manifold. In the case of non-equal diffusivities, the situation is more complex, but a similar (non-linear) invariant manifold can be obtained by an additional analysis of the eigenspaces of the diffusion matrix and full solution of (15). In other words, the system in (15) becomes linear, and therefore, any linear combination in the state space would be invariant under the degenerated system without the source term. Moreover, the fact that in the stationary limit the system solution is close to the so called mixing line allows us to use locally linear manifolds starting from the boundary

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domain till the initial/unburnt point. The term linear only means that the extended manifold locally belongs to a linear hyper-plane joining the boundary of the ILDM with the unburnt point (see Fig. 2).

Thus, by reaching during the generation the boundary domain between the two introduced domains, which is given or approximated by the limit of existence of the standard ILDM (a gap condition with user specified small parameter ε)

$$\Psi^* : \begin{cases} Re\left(\frac{\lambda_{m_s}}{\lambda_{m_s+1}}\right) \geq \varepsilon \\ \frac{1/\tau_{phys}}{Re(\lambda_{m_s+1})} \geq \varepsilon \end{cases}, \tag{12}$$

here λ_i are eigenvalues and τ_{phys} is the typical physical time scale, the manifold equation (4) is replaced by

$$P^\perp\left(\Psi_p\right)\left(I - V \cdot V^\perp\right)\left(\Psi - \Psi_{ub}\right) = 0. \tag{13}$$

Here $P\left(\Psi\right) = \begin{pmatrix} P_z \\ P_r\left(\Psi\right) \end{pmatrix}$, $P^\perp\left(\Psi\right)$ denote the parameterization matrix and its orthogonal complement, I - the identity matrix, Ψ_{ub} - the unburnt point and $V = \left(\Psi - \Psi_{ub}\right) \cdot e + T\left(\Psi_p\right)$, where e is the unit vector $e = (1,...,1)^T$, and $T\left(\Psi_p\right)$ is the local tangent space of the manifold boundary[14]. It can be shown by simple algebra that all points fulfilling (13) ly on the linear hyper-plane spanned by the cell boundary and unburnt point.

In other words, the tabulation procedure for the ILDM continuously checks the boundary condition (12) and thus identifies the boundary manifold (see Fig. 2). This condition normally reflects the situation when an additional chemical mode becomes slow and therefore the dimension of the slow subsystem has to be increased, which is normally the case in the boundary manifold. Then it continues to generate the manifold based on (13).

At this point, it is obvious that the questions of definition of the boundary manifold as well as determination of the minimal dimension of the slow manifold in the fast chemistry domain is a crucial point of the method and must be investigated before generating the matched manifold. Complete answers on these questions can not be given in the general case; they strictly depend on local properties of the considered model and on the accepted level of reduced model accuracy, but they can be obtained and controlled during the generation of the ILDM.

Finally, note that the use of grid coordinates θ with the projection defined by (10) is an ideal choice of reactive variables in both domains and, furthermore, the successive addition of cells is ideally suited for an ILDM generation. Furthermore, the generalized coordinates are very well adopted for an on-demand generation of the ILDM simultaneously with the CFD calculation. All terms necessary for subsequent use in the CFD calculation with reduced chemistry can be pre-calculated and stored during the generation of the ILDM if they are only functions of Ψ and θ respectively:

- the n by m_s-dimensional gradient of the manifold and its pseudo-inverse
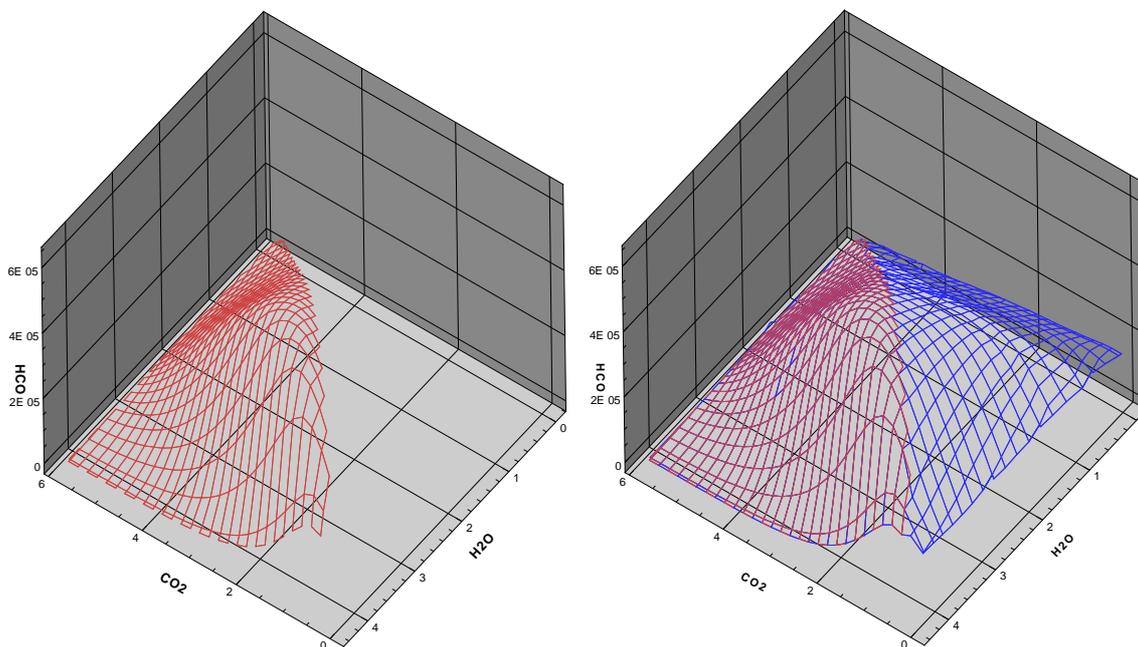
Figure 2: Treatment of the domain of slow chemistry: ILDM before (left) and after (right) extension.

- the chemical source term $F\left(\Psi(\theta)\right)$ is projected according to the reduced variables

- the projection matrix $Z_s \tilde{Z}_s$ for the transport term

In addition, besides the straight forward way described above, the hierarchical structure of ILDMs offers alternative methods to generate the manifold[15].

2.2 Projection of the governing equations

For an implementation of the developed method of system reduction into a reactive flow calculation it is necessary to derive reduced set of conservation equations. Let us start from a detailed equation system of a typical reacting flow process in symbolic vector form

$$\frac{\partial \Psi}{\partial t} = F\left(\Psi\right) - v \cdot \operatorname{grad}\left(\Psi\right) - \frac{1}{\rho} \operatorname{div}\left(D \cdot \operatorname{grad}\left(\Psi\right)\right) \tag{14}$$

where v represents the velocity field, ρ the density and D is the (n by n)-dimensional matrix of the transport coefficients[14, 16].

According to the basic assumption of the ILDM method, the state Ψ is, at any point of the flow and at any time, close to the manifold (i.e. the system dynamics in the state space are completely described as a movement within the manifold). If all thermochemical states everywhere in chemical reacting system are elements of the manifold, neither the chemical source term nor the convective term causes, by definition, movements in the

state space perpendicular to the manifold[3, 17]. However, a projection of the transport term is required and can be done by a transformation of the transport term into local coordinates of the invariant slow subspace

$$\frac{\partial \Psi}{\partial t} = F\left(\Psi\right) - v \cdot \text{grad}\left(\Psi\right) - \frac{1}{\rho} Z_s \tilde{Z}_s \cdot \text{div}\left(D \cdot \text{grad}\left(\Psi\right)\right). \tag{15}$$

Accordingly, the system (15) calculates the full n-dimensional state Ψ, but it restricts the evolution to a movement tangent to the manifold. Remind that $Z_s \tilde{Z}_s$ is the (n by n)-dimensional projection operator for the diffusion term. Now, the n-dimensional governing equation system (14) has to be projected to the m_s-dimensional reduced ILDM i.e. described by the generalized coordinates θ such that Ψ is assumed to be only a function of θ, which leads to the following representation

$$\Psi_\theta \frac{\partial \theta}{\partial t} = F\left(\Psi\right) - v \cdot \Psi_\theta \cdot \text{grad}\left(\theta\right) - \frac{1}{\rho} Z_s \tilde{Z}_s \cdot \text{div}\left(D \cdot \Psi_\theta \cdot \text{grad}\left(\theta\right)\right), \tag{16}$$

it is an n-dimensional equation system for m_s unknowns and, therefore overdetermined. In order to obtain the governing equation system in terms of the reduced variables the (m_s by n)-dimensional pseudo-inverse Ψ_θ^+ (10) of Ψ_θ is given by

$$\Psi_\theta^+ = (\Psi_\theta^T \cdot \Psi_\theta)^{-1} \cdot \Psi_\theta^T. \tag{17}$$

Ψ_θ^+ exists and can be found, if the m_s columns of Ψ_θ are linear independent vectors. Since the column vectors of Ψ_θ approximately corresponds to parameterization directions in the state space (7)-(10) linearly independence in Ψ_θ should be ensured. Multiplication of (16) with Ψ_θ^+ yields the equation system in terms of θ only

$$\frac{\partial \theta}{\partial t} = \Psi_\theta^+ \cdot F\left(\Psi\right) - v \cdot \text{grad}\left(\theta\right) - \frac{1}{\rho} \Psi_\theta^+ \cdot Z_s \tilde{Z}_s \cdot \text{div}\left(D \cdot \Psi_\theta \cdot \text{grad}\left(\theta\right)\right). \tag{18}$$

3 IMPLEMENTATION SCHEME

The ILDM table is generated in a pre-processing step, first the state vector Ψ, the chemical source term $F(\Psi)$, the matrices of slow invariant subspaces $Z_s(\Psi)$, $\tilde{Z}_s(\Psi)$ and an array containing several physical quantities (temperature, density etc.) are calculated at each mesh point as it was introduced in Section 2. The next stage is calculation of the terms $\Psi_\theta^+ \cdot F$, $1/\rho \, \Psi_\theta^+ \cdot Z_s \tilde{Z}_s$, and $D(\Psi) \cdot \Psi_\theta$ after finishing the generation of the ILDM, which are needed for the solution of (18), at each point of the generated ILDM table. This is possible, because of Ψ, Ψ_θ, D, Z_s and $\tilde{Z}_s$ are functions of θ only. Ψ_θ, the gradient of Ψ on the manifold, is approximated by central differencing and its pseudo-inverse Ψ_θ^+ is calculated as described above (17). Multiplication of Ψ_θ^+ with $F(\Psi)$ yields the m_s-dimensional projected source term $S(\theta)$

$$S(\theta) = \Psi_\theta^+(\theta) \cdot F(\Psi(\theta)).$$

The (m_s by n)-dimensional matrix $\Pi(\theta)$ projects the transport term onto the manifold and parameterize it to reduced coordinates. $\Pi(\theta)$ is given by multiplication of the matrix of right eigenvectors $Z_s(\theta)$ with the matrix of left eigenvectors $\tilde{Z_s}(\theta)$. A subsequent multiplication with $\Psi_\theta^+(\theta)$ yields

$$\Pi(\theta) = -\frac{1}{\rho}\,\Psi_\theta^+(\theta) \cdot Z_s(\theta)\tilde{Z}_s(\theta).$$

A multiplication of $D(\Psi(\theta))$ by $\Psi_\theta(\theta)$ yields the (n by m_s)-dimensional transport matrix

$$\Xi(\theta) = D\left(\Psi(\theta)\right) \cdot \Psi_\theta\left(\theta\right).$$

Thus, the reduced equation system can be rewritten as

$$\frac{\partial\theta}{\partial t} = S(\theta) - v \cdot \mathrm{grad}\left(\theta\right) + \Pi(\theta) \cdot \mathrm{div}\left(\Xi(\theta) \cdot \mathrm{grad}\left(\theta\right)\right). \tag{19}$$

Equation (19) is implemented and integrated in the 1-dimensional CFD code INSFLA[18]. It solves equations for mass, momentum, energy and the generalized coordinates under usage the ILDM table generated beforehand. The INSFLA reads the ILDM table and creates an initial profile over the spatial coordinate in terms of m_s-generalized coordinates θ. The partial differential equation system is described in space, and the resulting differential/algebraic system is solved by the implicit differential equation solver LIMEX[19]. The calculation of the right hand side is done by a finite differencing method. Within a loop over each spatial grid point the following steps are performed

- an interpolation in the ILDM table depending on the reduced coordinates θ is performed to get the terms $S(\theta)$, $\Pi(\theta)$ and $\Xi(\theta)$

- the m_s-dimensional term $\mathrm{grad}\left(\theta\right)$ is calculated

- the n-dimensional transport term $\mathrm{div}\left(\Xi \cdot \mathrm{grad}\left(\theta\right)\right)$ is computed and projected to the m_s-dimensional reduced manifold $\Pi \cdot \mathrm{div}\left(\Xi \cdot \mathrm{grad}\left(\theta\right)\right)$

- the m_s-dimensional convective term $v \cdot \mathrm{grad}\left(\theta\right)$ is calculated

- $S(\theta)$, $v \cdot \mathrm{grad}\left(\theta\right)$ and $\Pi \cdot \mathrm{div}\left(\Xi \cdot \mathrm{grad}\left(\theta\right)\right)$ are summed up to the right hand side

Additionally, since the mesh is locally orthogonal and equidistant and is, therefore, ideally structured for an efficient linear interpolation, a point-by-point search is not necessary. Finally, after finishing of each iteration step, a back-transformation of the solution in terms of reduced coordinates θ to detailed variables $\Psi(\theta)$ is performed by performing another interpolation in the ILDM table. This means that the primary results are spatial profiles of the generalized coordinates, and the species profiles can be recovered by a back-transformation (see Fig. 3).
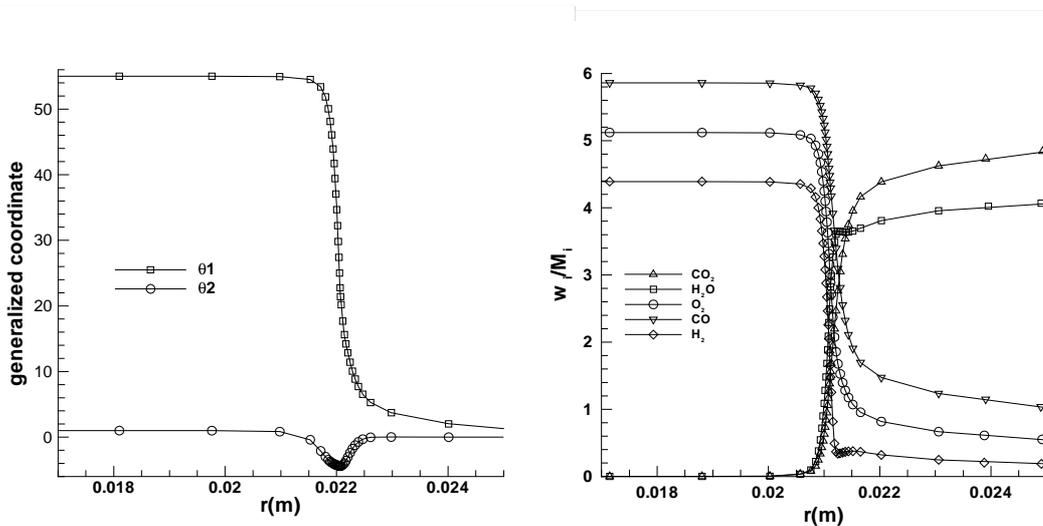
Figure 3: Stationary solution profiles in terms of generalized coordinates (left) and major species mole fractions profiles (right).

4 FLAME COMPUTATIONS AND DISCUSSION

In order to verify our method presented above, results obtained using detailed and corresponding reduced mechanism in terms of generalized coordinates are compared. Computations of adiabatic premixed syngas/air 1-dimensional free flames in a laminar flow field are performed [20, 21]. The unburnt mixture composition consists of $x_{CO} = 0.150$, $x_{O_2} = 0.131$, $x_{H_2} = 0.112$ and $x_{N_2} = 0.606$. Constant pressure, $Le = 1$ and equal diffusivities are assumed, but an extension to detailed transport models is possible without principal difficulties.

At first, $m_s=2$ is chosen as dimension of the reduced system (i.e. 2 generalized coordinates acts as reaction progress variables see Fig. 3. A 2-dimensional ILDM with corresponding element composition, pressure and enthalpy is generated and provided to the CFD code. In the free flame configuration Dirichlet conditions are used on the left boundary. The left boundary point corresponds to the unburnt point at 290K. On the right boundary, zero gradients are assumed (Neumann conditions). The regime of the 1-dimensional ILDM, starting with the unburnt point and ending up with the equilibrium point is used as initial profile. The results of the free flame computation are presented in Figures 4, 5. In Figure 4 concentration profiles of major species, in terms of $\frac{w_i}{M_i}$, are plotted versus the spatial coordinate and in a projection of the composition space.

Although a very small chemical mechanism (only 13 species) and a quite simple flow configuration is chosen, the economy of computational time is considerable. The reduced calculation requires only about fourth of the computational time to reach the stationary solution than the corresponding computation using the detailed mechanism. Figure 4 shows, that even the use of a 2-dimensional reduced mechanism yields accurate results

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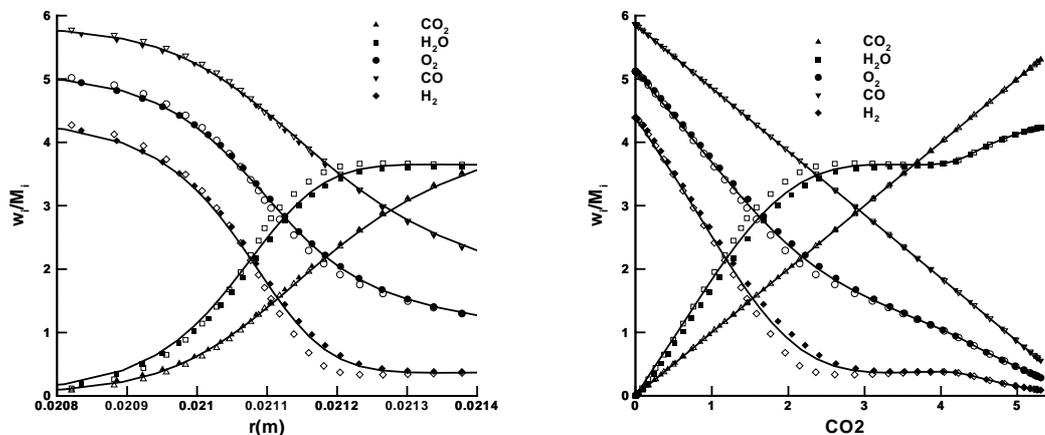
Figure 4: Comparison of major species of an unstrained flame solution using detailed kinetic model (solid lines), 2-dimensional reduced model (non filled symbols) and 3-dimensional model (filled symbols).

for the major species.

The boundary or the slow chemistry domain effect can be seen in Figure 4, which is rescaled Figure 3 (right) and corresponds to pre-heating zone in a flame or to the boundary domain in the composition space. In this domain more then 2 chemical time scales have become slow, such that they are of the order of magnitude of the physical processes. In Figure 4 (right) some major species are plotted against CO_2 molar fraction. The agreement is good, but in the boundary between the fast and slow chemistry, similar to the left figure, some deviations occur compared with the detailed mechanism (see the range of molar fraction of CO_2 from 1 to 3 in both right and left figures).

Figure 5 (left) shows the behavior of minor species - CH_2O over the spatial coordinate. It can be seen that a better description of those species can be obtained by increase of the ILDM dimension, in particular, 3-dimensional extended ILDM produces already not only qualitative but quantitative description. Figure 5 (right) illustrates that each additional reaction progress variable varies in a smaller range, it means the assumption of fast relaxation for the corresponding chemical processes is better and better fulfilled with increasing dimension.

5 CONCLUSIONS

A representation of ILDMs in terms of generalized coordinates together with a multi-dimensional extension procedure offer the advantage of a robust and efficient implementation. It is based on natural choice of the local manifold coordinates and on assumptions widely used in combustion theory. It is assumed, in particular, that there exists a sharp subdivision (splitting) of the state space into sub-domains with predomination of chemical kinetics or convection/diffusion terms. Accordingly, in the domain of fast chemistry the
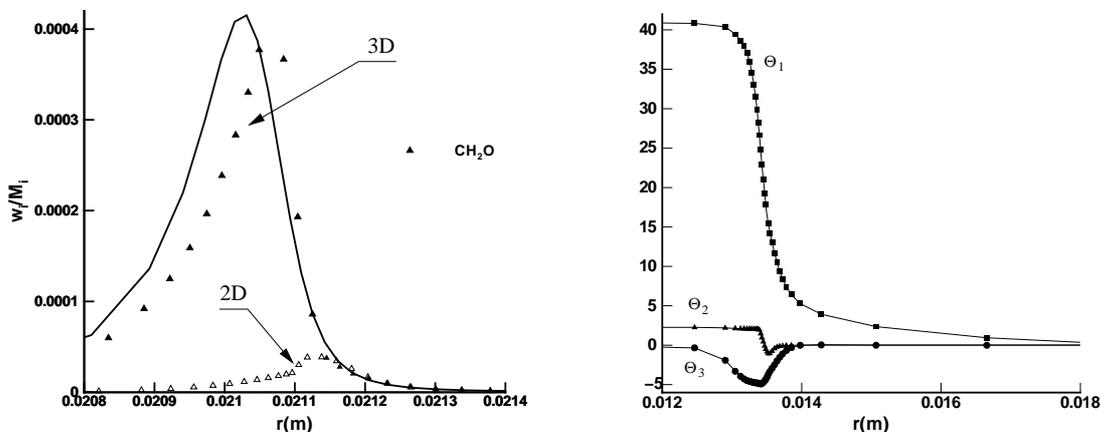
Figure 5: Mole fraction profile of CH_2O (left), comparison of detailed model (solid line), 2-dimensional and 3-dimensional reduced models and generalized coordinates profiles (right) for 3-dimensional reduced model.

standard ILDM method is used to approximate an invariant manifold of slow motions whereas in the no chemistry or low-temperature domain the locally linear extension of the ILDM and matching procedures have been proposed. It is suggested to increase the ILDM dimension to improve the performance of the ILDM near the boundary manifold. The reduced calculations yield a good agreement to the results obtained from the detailed calculation.

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