Validation of hierarchical REDIM based reduced models

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1 Introduction

Reliable modeling of chemical kinetics is a challenging task in the development of combustion models. To cope with this problem and to reduce computational costs the manifold based model reduction strategy has become a valuable tool in simulations of combustion processes, especially in turbulent combustion [1]. It has various advantages in implementations - a very low dimensionality of the resulting reduced models on one hand side and a very high accuracy of the applications on the other. Moreover, because of the tabulation the whole thermo-chemical state space of a combustion system is accounted for, meaning that all important information on particular species is considered.

In the present study crucial problems of model reduction by manifolds methods are discussed. Three main problems related to (i) accuracy, i.e. how many dimensions to implement to describe e.g. transient regimes reliably; (ii) boundary definition, how to define what part of the system's state space should be accounted for; (iii) construction, how to construct the manifold of required dimension within the specified range / domain are treated with a main emphasis on validation (i) of manifolds based reduced models. Typically, in many applications all these questions are either omitted completely or they are treated empirically, i.e. dimensions and domains for which the states are tabulated are postulated.

The hierarchical structure of the manifold (with respect to dimensionality [2]) together with a suitable distance defined in the system's state space and geometrical interpretation of the boundary of the manifold allow to overcome most of the problems with construction and with applications of the manifolds based reduced models.

For this purpose the Reaction-Diffusion Manifolds (REDIM) [3] method is further developed to perform a generic and fully automatic construction of REDIMs reduced models. Free premixed flames with detailed chemical kinetics are considered to illustrate and verify the proposed approach.

2 Problem statement and suggested solution

Within the manifolds based model reduction, states of the detailed combustion system are considered to cover not the whole thermo-chemical systems state space, but they are restricted to a low dimensional

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manifold. The system's degrees of freedom, as a number of variables to be taken into account are restricted to the dimension of the manifold.

A very common approach to construct such a manifold is by using several stationary / in-stationary detailed solution profiles. Thus, a transient system behavior then is described by a few progress variables and/or the mixture fraction (see e.g. [4]) along these profiles. This, however, requires very detailed *a priori* information about the system. Moreover, in this way it is not easy to increase the manifold dimension. This drawback becomes especially apparent in the case of premixed laminar flames for which only a one stationary solution can be found. This solution can be represented by only one-dimensional profile (curve) in composition space.

Accordingly, in order to be able to implement efficiently the manifold based model reduction one needs to define the dimension, boundaries and location of an appropriate manifold in the system state space. In the following sections, first, the *distance* in the system state space is suggested to quantify the quality of model reduction for a fixed dimension. Then, the problems of the manifold boundary and of construction are treated generically by using the hierarchical nature [2] of the system invariant manifold [5] and by implementing the REDIM concept (see e.g. [6]). This altogether gives us possibility to devise an algorithm to develop reduced models of arbitrary dimension that can be implemented full automatically.

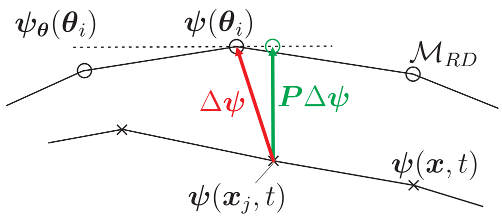
3 Accuracy of the reduced model

It is obvious that the solution for the first problem cannot be given in general, but it has to be problem specific. Typically, in order to verify and validate a reduced model detailed and reduced systems solutions are compared in post processing for e.g. particular species profiles or by comparing the performance of both models with experimental results (using ignition delay times, extinction limits etc.). In this way manifolds can be indirectly verified. Consider now, a combustion system state vector Ψ on a manifold M. It can be assigned to the coordinates of the parametrization $M = \{\Psi = \Psi(\theta) | \Psi : \mathbb{R}^m \to \mathbb{R}^n, m << n\}$ where Ψ is the ($n = n_s + 2$)-dimensional thermo-chemical state vector, n_s species number, M is the manifold of dimension m and $\theta = (\theta_1, ..., \theta_m)$ is the vector of the local coordinates [3].

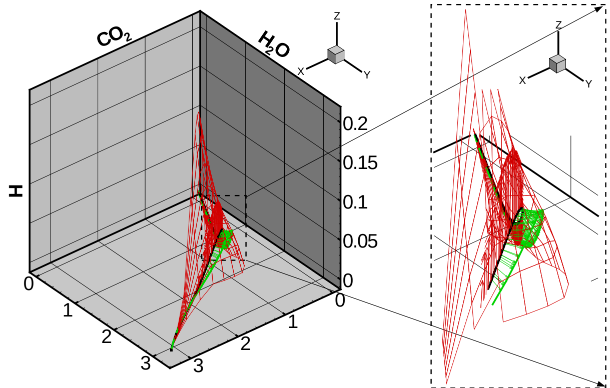
In the current work, for validation of the manifold the following distance in the system state space is suggested, which is suitable for discrete representation of the solution profile as well as for the manifold itself. Thus, at any point of the detailed system solution $\Psi(x_i, t)$ one evaluates

$$\rho(\Psi(x_i, t), M) = \| Proj_{NM} \left(\Psi(\theta^*) - \Psi(x_i, t) \right) \| . \tag{1}$$

Figure 1a shows schematically the realization of the distance to access the quality of the reduced model, where $Proj_{NM}$ is the local projection onto the normal space of the manifold at $\Psi(\theta^*)$, $\Psi(\theta^*)$ is the closest point of the manifold discrete representation to the point on the detailed solution $\Psi(x_i, t)$ and $\|...\|$ is the euclidean norm. Note that a scaled norm can also be used without any difficulties. In order to obtain the final distance one should calculate the average of distances at all points of transient system solutions to make the measure independent on the number of points in the discrete representation. It is very important to note that the suggested distance can be also applied as a measure of distance between two low-dimensional manifolds of arbitrary dimension.



(a)



(b)

Figure 1: (a): Scheme of the distance estimation between the detailed solution profile $\Psi(x,t)$ and a manifold $\Psi(\theta)$; (b): An instant of the transient solution profile (black curve) shown in the projection to $\mathrm{CO_2} - \mathrm{H_2O} -$ H, specific mole numbers, 1D REDIM (green curve) and 2D REDIM (red mesh) are shown with vectors signifies the distances to corresponding manifolds.

4 Reduced model analysis

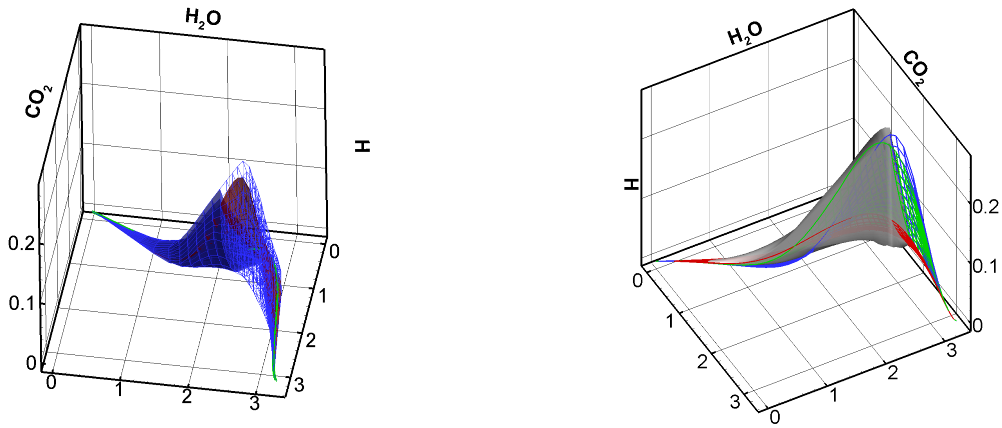
Now, in order to present the suggested approach a free laminar premixed syngas-air system is considered. The premixed composition consists of 0.5 mole CO, 0.5 mole $\mathrm{H_2}$, 1 mole $\mathrm{O_2}$ and 3.762 mole $\mathrm{N_2}$. That is, combustion system as a lean syngas mixture with air is considered.

In order to test the performance of a reduced model for a transient system behavior the so-called triple map perturbation of the one-dimensional turbulence theory [7] is used. In this case the system's stationary profile is taken and the reaction front is cut into three parts, which are redistributed in space such that the middle one is defined by reflection about its center line. The solutions in two external parts is re-scaled to match the boundaries of the changed middle part yielding continuous profile [7]. The latter can be taken as perturbed initial condition for testing. In this way the perturbed initial profile follows the same path in the state space, while in the physical space the profile is strongly perturbed compared to the stationary solution. System solution gradient estimates are tripled instantly, causing a rise in the influence of diffusion processes and thus disturbing the equilibrium of the stationary profile. This can serve as an extreme example of a turbulent vortex acting on the combustion flame front.

Figure 1b shows the typical distance vectors from the detailed system solution profile (black curve) to corresponding 1D and 2D REDIMs after the triple map functional transformation has been implemented and while the system solution returns to its stationary profile. The distances are calculated at a particular integration time t_0 and arrows show distance vectors of this instant of the transient solution profile to corresponding manifolds.

Hierarchical implementation of the REDIM

The main assumption of the REDIM model reduction concept is the invariance condition [3, 5]. Namely, it is assumed the stationary solution as well as the transient system solution profiles are confined to a REDIM



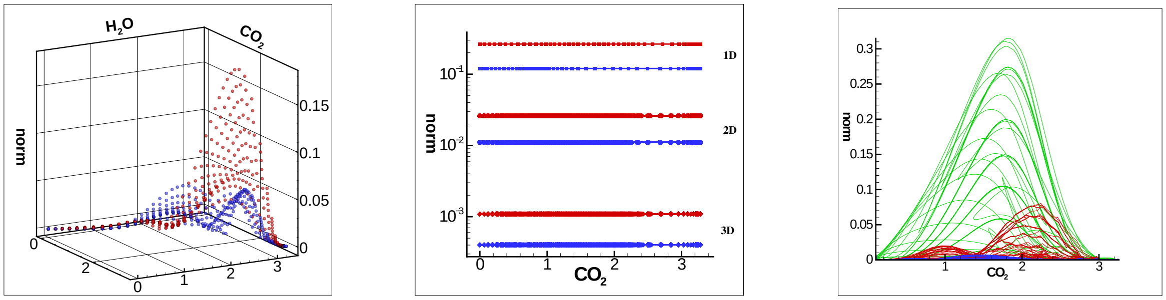
(a) (b)

Figure 2: Hierarchical construction of the REDIM in $\mathrm{CO_2 - H_2O - H}$ projection, (a): 1D (green curve), 2D (red mesh), and 3D (blue mesh) REDIMs; (b): 3D REDIM (gray filled sleeve) manifold and three different 2D REDIMs, green mesh shows the standard 2D REDIM, red mesh was generated with doubled gradient estimates taken from the stationary solution as for the green one, while blue mesh represents the 2D REDIM for halved gradient estimates.

of a certain dimension at any time and spatial location. In a previous work [6] a hierarchical construction was introduced and now it is extended to the 3D case. Figure 2 (a) shows the hierarchical construction of the REDIM manifold starting from 1D (green line) and extending to 2D (red mesh) and 3D (blue mesh). Due to the internal hierarchical structure of the invariant low-dimensional manifolds [2] and due to appropriate boundary conditions [6] the dimension increase of the reduced model has become generic and can be performed fully automatically. Because the 1D REDIM corresponds to the stationary profile and has to be a part of 2D REDIM (for the same gradient estimates see e.g. [2]), it can be used as a basis for construction of the 2D REDIM where an additional dimension is added by using slight perturbation to the gradient field and extension procedure with suitable reparametrization [6]. Afterwards, when the 2D REDIM is constructed one can follow the same procedure to extend 2D REDIM by one dimension only to 3D REDIM (blue mesh in Fig. 2 (a) and gray sleeve in Fig. 2 (b)) etc. Once manifolds of different dimensions are constructed we can start to compare and to study their properties.

Gradient dependence

Another interesting application for the suggested distance is a comparison of different manifolds. The distance can be used to access the sensitivity of the manifold to system parameters and to check assumptions made e.g. for diffusion terms, i.e. their weak sensitivity to gradient estimates. Indeed, during the REDIM generation process different gradient estimates can be used to generate the manifold [3], however, as it was stated in our previous works the sensitivity of the manifold vanishes with the increase of the reduced system dimension. Now, we are able to quantify this by using the distance Eq. (1) and different gradients' estimates. Figure 2 (b) shows three different 2D REDIMs constructed for gradients taken from the stationary system solution (shown by green mesh) together with doubled (red mesh) and halved (blue mesh) gradient



(a) (b) (c)

Figure 3: Pointwise distances between the REDIMs and between transient profile and REDIMs. (a): distances in $\mathrm{CO_2} - \mathrm{H_2O} - \mathrm{norm}$ - projection between the standard 2D REDIM (green mesh in Fig. 2(b)) and two 2D REDIMs with changed gradient estimation (blue and red meshes in Fig. 2(b)); (b): same as in (a), but average distances in $\mathrm{CO_2} - \mathrm{norm}$ - projection between 1D, 2D and 3D REDIMs are shown in logarithmic scales; (c): same projection as in (b), distances between the detailed systems solution profiles as a consequence of relaxation after triplet map implementation and 1D (green), 2D (red) and 3D (blue) standard REDIMs are shown.

estimates. One can see that in this projection (this is still true in any other projection) all three 2D REDIMs located within the same standard 3D REDIM (with gradient estimates taken from the stationary solution).

In the present work, because of the premixed case a simple but transparent euclidean norm is employed in Eq. (1) and it is calculated for specific mole numbers. This is only to visualize the trend of the decrease in distance depending on the dimension considered. However, the suggested measure can be modified for particular application and can yield estimation for relative and quantitative deviations of the reduced and detailed solutions as well as for manifolds.

Figures 3(a,b) show distances between the manifolds for different gradients estimates. Figure 3(a) represents the pointwise distance between the standard 2D REDIM green mesh (in Fig. 2(b)) and two other 2D REDIMs constructed for larger (red) and smaller (blue) gradient estimates. One can see the manifold with halved gradients estimates deviates less than that with doubled gradients estimates. This trend is true for 1D as well as for 2D and 3D cases. Figure 3(b) shows average distances between corresponding manifolds for three 1D, 2D and 3D cases in all cases smaller gradients shows weaker sensitivity to gradient estimates, while with increasing the dimension distance between perturbed manifolds and standard ones decreases by an order of magnitude.

Figure 3(c) shows transparently the same trend, where the transient solution profiles after the triple map perturbation is integrated and the distance between the instant profiles for several time steps and corresponding manifolds is calculated. After the perturbation, the profile starts to deviate from the stationary system solution (green curve in Fig. 1b and in Fig. 2(a)), which results in large maximal values of the green curves in Fig. 3(c). Then with time the solution profile will return back to the stationary systems solution, thus, the distance have to vanish with the time. Moreover, the quality of the reduced model can be accessed by comparison of maximal values for manifolds of different dimension. One can see that the red curves have lower maximum as a green ones, while blue curves almost vanish and appears mainly due to discretization error.

5 Conclusion

In the present work some important problems of manifolds based model reduction were discussed. The problem of reduced model accuracy and its validation was in the focus of the study. The approach to quantify the accuracy of the reduced model in the system state space was suggested. It is based on the euclidean distance and is suitable for pointwise discrete representation.

A slightly lean free premixed syngas-air flame was considered for illustration and verification of the suggested approach. A 3D REDIM manifold is constructed and results of 1D, 2D and 3D reduced models were presented.

The study shows that the suggested approach can be used successfully to verify the accuracy of the reduced model and to study properties and sensitivity of the manifold to system parameters. In particular, it was demonstrated that the 3D REDIM for the considered combustion system is not sensitive to perturbations of the gradient estimates and it completely describes the transient system behavior after a strong triple map perturbation was applied. The latter means that the constructed 3D REDIM manifold can be used efficiently to study premixed turbulent flames.

Acknowledgments

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