An improved tabulation strategy for reduced chemical kinetics based on ILDM

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Abstract

In order to simulate practical combustion processes simplified models for both, the turbulent flow field and chemical kinetics are necessary. In this work our focus is on the simplification of the chemistry using the ILDM (Intrinsic Low Dimensional Manifold) method. In order to improve the accuracy of the reduced scheme locally high dimensional ILDMs are desirable, which on the other hand leads to a large amount of storage. However, in applications the accessed domain of the ILDMs is much smaller than the whole allowed composition space. Therefore, an automatical identification procedure was developed in order to obtain the boundaries of the domain representing the actual accessed space. The method used is based on a multi–dimensional continuation procedure. The convex domain is identified based on an analysis of the chemical and physical processes. The advantage of this method is that no further simplifications of the reduced scheme is made, i.e., the whole information needed for numerical simulations of reacting systems is still available.

Introduction

For the numerical simulation of practical combustion processes simplified models for both, chemical kinetics and the turbulent flow field have to be used. Otherwise the CPU–times needed exceed available resources even on todays supercomputers. In this work we present some new aspects of the method of intrinsic low–dimensional manifolds (ILDM) for the simplification of the chemical kinetics (see [1]). This approach is based on a local time scale analysis of the Jacobian of the chemical reaction system. Starting from the detailed chemical rate equations, it identifies attracting m–dimensional ILDMs in the n–dimensional state space having the property that after a short time interval the thermochemical state of the system has relaxed onto the manifold. These ILDMs are pre–calculated and stored, and then all information on the chemical kinetics is available using a simple table look–up procedure.

Basically the method of ILDM consists of three steps, namely the identification of the intrinsic low–dimensional manifolds, the storage of the results and the solution of the reduced equation system for the scalar field. A robust numerical method for the calculation of the ILDMs has been developed [2]. It is based on a multi–dimensional continuation procedure which yields the ILDM in terms of a locally adapted parametrization. Furthermore, a method has been developed which allows to express the precalculated ILDMs in terms of a fixed set of reaction progress variables [3].

One remaining problem is the large amount of storage needed to tabulate the ILDMs. This is particularly important if high local dimensions of the ILDMs are necessary due to accuracy aspects like, e.g., in the simulation of ignition processes. It is, however, well known that the state space accessed in typical applications is confined to a small subset of the state space (see, e.g., [4]). Thus, an enormous reduction of the storage requirement can be achieved if the actually accessible space is identified during the calculation of the ILDMs and the ILDM is stored only for this subdomain of the whole composition space. In this work we present a procedure to identify the boundaries of the accessed domain of the ILDM automatically.
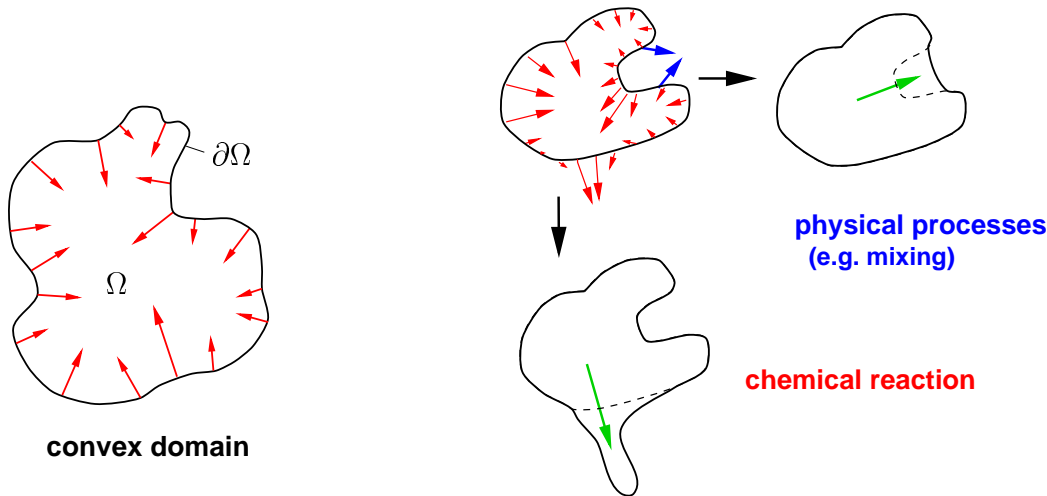
Figure 1: left: convexity of the ILDMs, right: scheme of the automatic build up of the convex domain.

Automatically identification of the accessed domain

In the following we will call the domain Ω of the ILDM convex if no chemical or physical process can cause a movement in the state space which leaves the domain of the manifold, i.e. if all possible rates of change on the boundary $\partial\Omega$ of the domain are zero or are directed into the domain Ω (see Fig. 1 left). Convexity in the context of the ILDMs is based on the behavior in the local tangent space after the chemical and physical processes have been projected onto the manifold.

Having identified the convex domain, it is guaranteed that all points in state space actually accessed lie inside the convex domain. This means that during the calculation of the manifold starting, e.g., from the equilibrium value, a continuous check of the processes at the boundary has to be performed. If both physical and chemical processes on $\partial\Omega$ are directed into the domain Ω, there is no need to increase the domain Ω, but if either the physical or the chemical processes are directed out of the domain, the domain Ω has to be increased in this direction (see Fig. 1 right).

Whereas for the chemical kinetics the rates are unique functions of the composition (i.e. they are explicitly known on the boundary $\partial\Omega$), the rates of change of the physical processes (diffusion, molecular mixing, etc.) depend on the system under investigation and have to be adapted to the specific problem considered. For a molecular mixing process, e.g. in PDF calculations, the direction of molecular mixing between two points on the manifold is obtained by projecting the vectors of mixing $(\Psi^1 - \Psi^2)$ onto the manifold.

This procedure of building up a convex domain can be implemented into the multi–dimensional continuation method in order to determine the accessed subspace. In this method the parametrization mesh is built up by a successive addition of cells [2]. In order to guarantee the convexity of the manifold each cell has to pass several steps before it is added. The directions in which cells are added are determined by the mixing processes, e.g. mixing between neighbouring cells, mixing with the unburnt mixture, diffusive processes, etc., and the chemical reaction progress.

This is exemplified in Fig. 2 (left). The dotted arrow denotes the direction of the physical perturbation. Furthermore, at each corner of the cell the chemical directions (grey arrow) are determined.

Using the new parametrization strategy cells are added, if the process vector points outside the cell (i.e. here the cells 1,3 and 4 are added, but not cell 2). In this way the result is a convex domain (Fig. 2 right). All direction vectors (arrows) on $\partial\Omega$ point into the domain Ω itsself.

Because of the fact that the accessed space is only a small fraction of the overall composition space the storage requirement of higher–dimensional manifolds does not increase as extremly with the dimension as expected for conventional tabulation strategies ($2^{\dim}$). This is particularly important for higher dimensional manifolds because the storage requirement for the tabulation of the ILDM for subsequent use in CFD codes is decreased considerably. Furthermore, restricting the accessed domain is no simplification of the chemical system, but it is only a reduction of the tabulation area by focusing only on the relevant subspace.
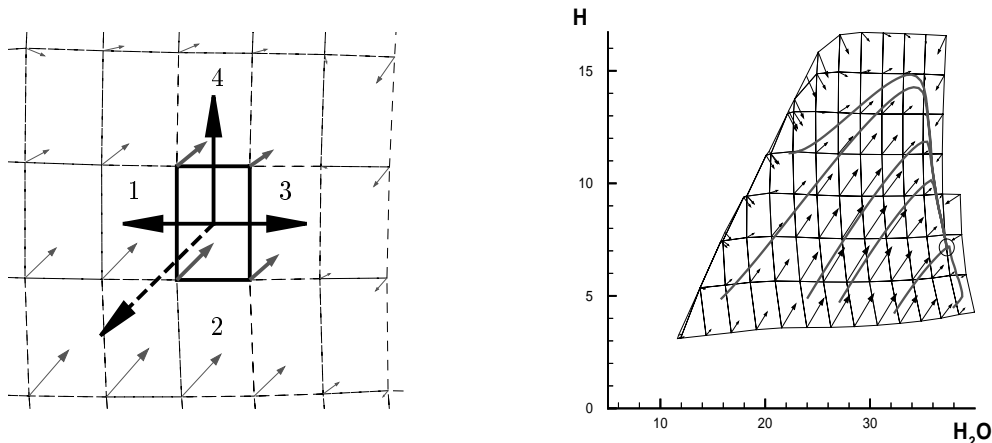
Figure 2: left: schematic illustration of the cell addition; physical direction (dotted arrow), chemical directions (grey arrows) and resulting directions of the cell addition (black arrows), right: resulting convex ILDM, trajectories (grey lines) correspond to the reaction progress.

Implementation in CFD codes

The implementation of the ILDMs in CFD codes is done using a simple look–up table in which the ILDM is mapped onto a subspace spanned by reaction progress variables [3]. This approach has already been verified by various laminar and turbulent flame calculations [4–6]. Also validation calculations have been performed for the new procedure.

Conclusions

The presented method allows to identify automatically the boundaries of a convex ILDM independent on a specific application. The only input for the tabulation procedure is the detailed chemical reaction mechanism and the required dimension of the simplified scheme. The essential advantage of the method is that the storage requirements decrease without loosing any information in the accessed domain and without any further simplification of the reduced scheme. This is an important fact because higher dimensional tables of the reduced kinetics can then be used with a reasonable amount of storage requirements for the look–up tables of the ILDMs. Higher dimensional manifolds will increase the accuracy of chemical kinetics for the simulation of various practical applications like, e.g., ignition processes, where locally fast timescales can become important.

Acknowledgments

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