On the spatial dependence of REDIM based reduced models for modeling of reacting flows

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Abstract—**The method of reaction-diffusion manifolds (REDIMs) presents a very attractive and efficient tool for model reduction of reacting flows. The method is designed to take into account and employ the information both about detailed chemical kinetics and about molecular transport. The method uses attracting low-dimensional manifolds defined in the composition state space of a reacting flow system. In the current work spatial dependence of the REDIM manifold is studied. The problems of identifying a suitable manifold dimension, devising conditions for the evolution of the boundary and estimating the gradients are discussed in detail.**

I. Introduction

Reacting flows are governed by a complex interplay of chemical reaction, flow, and molecular transport. They can be described mathematically based on conservation equations for mass, momentum, energy, and species masses. In the vector form the system comprises the chemical source term, the advection and the diffusion terms correspondingly:

$$\frac{\partial \psi}{\partial t} = F(\psi) - \vec{v}\,\mathrm{grad}\,\psi + \frac{1}{\rho}\mathrm{div}\left(D(\psi)\mathrm{grad}\,\psi\right). \qquad (1)$$

The system state vector $\psi = \left(h, p, w_1/M_1, \ldots, w_{n_s}/M_{n_s}\right)$ is a vector of $(n = n_s + 2)$ dimensions composed of the thermodynamic and of the composition space [1]. F is the chemical reaction source term, $\vec{v}$ is d-dimensional velocity vector, ρ is the density and D is the matrix of diffusion coefficients.

One major problem of (1) is that the description of chemically reacting systems leads very often to reaction mechanisms with far above hundred chemical species (and, therefore, to more than a hundred partial differential equations $n_s \sim O(100)$). These kinetic processes cover time scales from nanoseconds to seconds. An analogous scaling problem arises for the length scales. The scales of technical systems may be several meters, and on the other hand, typical reaction zones or small turbulent structures have length scales of the order of millimeters. Due to these scaling problems, the system of partial differential equations (1) represents a highly stiff system. Thus, the detailed simulation of three-dimensional turbulent flows in practical systems is beyond the capacity of even today's supercomputers. Because the use of simplified sub-models is the only way out of this problem the interest in automatic approaches that reduce the dimension and complexity of the system without quantitative loss of the accuracy has increased over the last decades [2-6].

II. Problem statement and toy example

In general, efficient methods to simplify the description of the chemical kinetics answering the question above can be devised if one makes use of the fact that

- not the whole composition space (spanned by e.g. the large number of species concentrations) is actually accessed; and
- the dynamics is confined to low-dimensional manifolds in composition space.

The problem of model reduction reduces then to the problem of definition of such manifolds which describes the evolution of the detailed system in the physical space by/through the parameters of the manifold only. Therefore, the dependence of the manifold on space represents a very important and not yet sufficiently investigated topic of model reduction. In order to attack this problem let us investigate first the evolution of a reaction/convection/diffusion system. In a general d-dimensional flow the thermo-kinetic state ψ is a unique function of the d-dimensional vector r of spatial coordinates and the time t:

$$\psi = \psi(r, t).$$

Note that this unique mapping defines at a certain initial time $t = t_0$ a manifold in composition space (in order to simplify the treatment we assume that complex topological structure can be split into piecewise defined manifolds). These manifolds have the following properties:

- they have a maximum dimension of 3 ($d \le 3$ three spatial coordinates),
- the mapping is not injective (the same state vector can be found at different spatial locations,
- boundaries in the physical space do not need to correspond to boundaries in composition space.

This can be visualized by a simple3D toy system ($n = 3$) in an artificial two-dimensional ($d = 2$) physical space

$$\psi(x, y; t_0) = \begin{pmatrix} \sin(2\pi x)\sin(2\pi y) \\ y \\ \sin(2\pi x)\cos(2\pi y) \end{pmatrix}, \quad x \in [0,1],\ y \in [0,1]. \qquad (2)$$

This system is plotted in physical space (Fig.1, left) and composition space (Fig. 1, right). This simple example shows clearly that the physical boundary does not correspond to a boundary of the manifold in the composition space. Therefore it is important to know how the boundaries

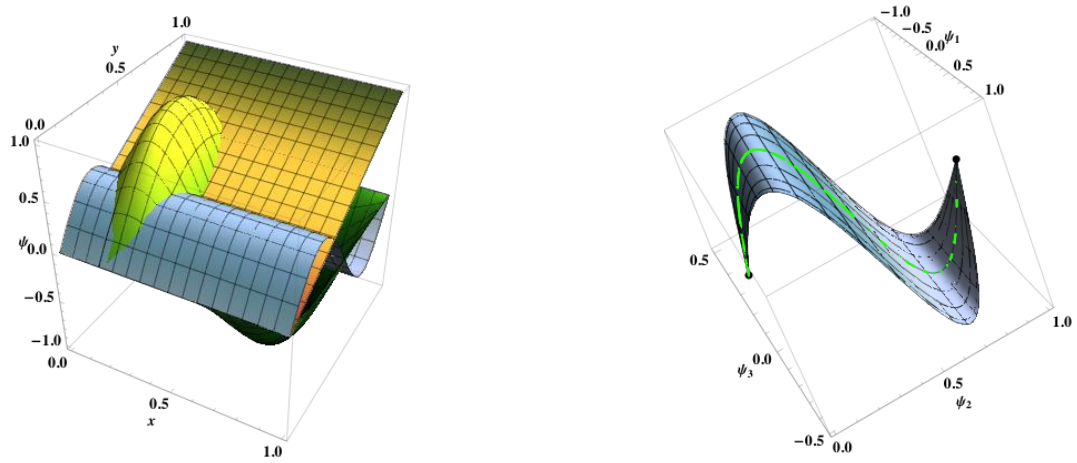

Fig. 1 Left: Plot of the toy example in physical space; blue: ψ_1, yellow: ψ_2, green: ψ_3. Right: Plot of the toy example in composition space, surface: low-dimensional manifold, green curve: boundary points in physical space.

of the manifold evolve in time, and how the physical dimension maps to the manifold dimension.

III. REDIM

The method of reaction-diffusion manifolds (REDIM) [7-11] approximates the dynamics of the detailed system (1) in the composition space. It solves an evolution equation for the manifold based on an initial guess (where the dimension is already prescribed) and on an estimation of the local gradients, assuming that the gradients are unique functions of the thermo-kinetic state. Thus, while looking at the simple toy example shown above several important questions arise:

1. How can the reduced model dimension be defined? In this work we show how the information about the system gradients in the compositions space can be used to answer this question.
2. How can the boundary (and its evolution) in composition space be described? We show that at the boundary of the manifold the component of the gradient in physical space tangential to the manifold and perpendicular to the boundary vanishes. This allows us to devise an evolution equation for the boundary of the manifold.
3. How well is the dynamics characterized by a gradient estimate that depends only on the location in the composition space and not on the location in physical space? It is evident that if one point in composition space can correspond to different points in physical space, then in reality the gradient is not a unique function of the location in composition space. Therefore we discuss the influence of the gradient estimate on the evolution of the manifold.

IV. CONCLUSIONS

In spite of the progress made in the development of the REDIM model reduction strategy, there are several very difficult and complicated issues concerning the spatial dependence of the manifold. The simplest and most obvious way to solve this problem is to postulate "complete" independence of the manifold on the spatial phenomena. In this study, however, we show how these problems can be handled in a more sophisticated way.

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