HIERARCHICAL CONCEPTS FOR MODEL REDUCTION FOR REACTING FLOWS BASED ON LOW-DIMENSIONAL MANIFOLDS

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Abstract

The evolution of the vector of scalars (enthalpy, pressure, species concentrations) of a reacting flow is governed by a partial differential equation system of the form

$$\frac{\partial \psi}{\partial t} = F(\psi) + \nu \cdot \operatorname{grad} \psi + \frac{1}{\rho} \operatorname{div} D \operatorname{grad} \psi \,.$$

where ψ is the $(n_s + 2)$ dimensional vector of thermokinetic variables (n_s = number of chemical species), $F(\psi)$ is the vector of (chemical) source terms, ρ is the density, ν the flow velocity, and D the matrix of transport coefficients.

The description of chemically reacting systems (e.g. combustion, chemical processes in the atmosphere, or biological systems) leads very often to reaction mechanisms with far above thousand chemical species (and, therefore, to more than a hundred partial differential equations), which possibly react within more than several thousands of elementary reactions. These kinetic processes cover time scales from nanoseconds to seconds. Due to these scaling problems the detailed simulation of three-dimensional turbulent flows in practical systems is beyond the capacity of even today's super-computers. Using model reduction concepts is a way out of this problem.

Both the chemical source term and the molecular transport term have one important property, namely that they cause the existence of low-dimensional attractors in state space (the space spanned by the thermokinetic variables). These manifolds can be parameterized by a small number of variables, and the original evolution equation can be projected onto those low-dimensional manifolds.

In this work we discuss several model reduction aspects based on the concept of low-dimensional manifolds, namely the efficient identification of the low-dimensional manifolds, the efficient implementation to simplify the chemical kinetics, the hierarchical nature of the low-dimensional manifolds, and the use of the model reduction in reacting flow calculations.