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Sensitivity analysis and mechanism simplification using the G-Scheme framework

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ABSTRACT

We have developed specific procedures that utilize the G-Scheme modal decomposition to carry out the sensitivity analysis along-with the numerical integration of chemical kinetics systems, so as to understand the roles of the most important reactions, and to identify the most important reaction paths of the processes. The sensitivity information allow to generate skeletal kinetic mechanisms for chemical kinetics mechanism. The procedures are based on participation indices constructed from the G-Scheme dynamics decomposition, but can be applied to databases generated by any numerical solver. The effectiveness of these procedures is demonstrated with reference to the auto-ignition problem of a homogeneous hydrogen/air mixture.

1. Introduction

The development of combustion models is key for the design of advanced engines [1]. In reactive flows, chemical reactions and fluid dynamics are tightly coupled, so that the heat released drives or alters the fluid motion. The interaction between reaction, advection, and diffusive processes involves a broad range of scales. This aspect, and the high resolution demanded [2], makes reactive flow problems impractical to solve even using high performance computers and dynamically adaptive numerical methods [3,4].

Detailed chemical reactions mechanisms involve a large number of species and reactions [5]. The use of a simplified model is a common simplification, although it may introduce significant errors in the simulation. As an example, phenomenological models such as one- and two-step reactions are not able to capture all relevant dynamics inherent in the full mechanism, so that the simulations are only qualitatively representative of the physical phenomena [6]. The computational cost of a calculation of a single time step for kinetic schemes typically scales linearly with the number of reactions, and quadratically with the number of species [7]. Therefore, a saving in CPU time and memory overhead required to solve reactive flows with detailed kinetics can be achieved by reducing the number of species and reactions in the detailed mechanism. The construction of simplified reaction models is an active field of research [8–10].

There exist methods, such as Computational Singular Perturbation (CSP) [11,12], the G-Scheme [13], the multi-timescale (MTS) method, and the hybrid multi-timescale (HMTS) method [14], that use different numerical strategies to reduce the computational cost. A variety of other methods have been proposed over time, some of them with the goal of producing a number of global reaction steps, while others aim at trimming non-important species and reactions from the detailed mechanism. For example, the method of sensitivity analysis (SA) [15] investigates the effect of parameter change on the solution of mathematical models. Though it does not directly provide decoupled information about the reactions and species, the interpretation of sensitivity coefficients provides information on the importance and interconnections of parameters and variables. Other notable examples are the method of principal component analysis (PCA) [16] and the Direct Relation Graph (DRG) method [17]. The PCA, based on SA, systematically identifies the redundant reactions by operating on the sensitivity matrices. The DRG aims at reducing the number of species and eliminates the elementary reactions associated with them within a specified accuracy requirement.

Model simplification methods aim at modifying the detailed kinetics by trimming the species whose kinetics are not tightly coupled with those of interest as well as the reactions judged unimportant to the retained species. The outcome of this procedure is a smaller kinetic mechanism which is a subset of the detailed mechanism. By construction, this skeletal mechanism is supposed to be

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accurate only with respect to the species declared of interest and if it is used inside its domain of applicability.

Some simplification methods use parameters to estimate the relative importance of reactions. These parameters are constructed by manipulation of the production/consumption term relating the kinetics of individual species. In particular, the simplification procedure based on CSP [7] introduces a set of fast and slow importance indices aimed at identifying the processes that produce the most significant contribution in either the fast or slow components, so as to select them to form a skeletal mechanism. This is obtained by the ability of the CSP method to decompose the chemical kinetic processes into fast and slow components, respectively. More in detail, this procedure introduces an algorithm that evaluates the relevance of a subset of reactions within fast or slow dynamics of a prescribed set of kernel species. Both the fast and slow dynamics of the kernel species are accurately reproduced by the skeletal mechanism.

The present work focuses on the G-Scheme sensitivity analysis, its definition, its applicability for understanding chemical kinetics, and its ability to identify a of simplified mechanism. The simplification procedure is explained in detail, highlighting its dependence only on the accuracy required by the user for the simplified mechanism. In order to better clarify these aspects, we initially recall the main features of the G-Scheme. Subsequently, the current work presents a new index based on the G-Scheme features that allows one to identify the most important reactions driving the kinetics of the combustion process. This index provides, in addition, information on the role of the reactions during the complete process. Moreover, using a global definition of the index we develop a simple procedure that creates several skeletal mechanisms able to reproduce qualitatively and/or quantitatively combustion processes. With this objective methodology the user creates simplified mechanisms simply by selecting the admitted error on one or more quantities of interest. The simplified mechanism obtained serves the double purpose of a computationally affordable mechanism for computational fluid dynamics simulations and skeleton mechanism for sensitivity analysis containing all the essential information to investigate the physics behind the combustion process. We discuss in detail the procedure to obtain the simplified mechanism.

The auto-ignition of a hydrogen/air homogeneous mixture is used to illustrate the methodology in order to show the effectiveness of the analysis as well as the simplification procedure. Successively, the G-Scheme analysis is applied on the simplified mechanism in order to understand the roles of the reactions and analyze the chain-branching sequence. The analysis for the explosion regime and the roles of positive eigenvalues are also exposed. Finally, the simplified mechanisms as well as the eigenvalues analysis are discussed in light of other works published in the literature.

2. The G-Scheme method

The numerical solution of multi-scale models is a challenging task because of the simultaneous contribution of a wide range of time scales to the system dynamics. However, it is typical that the dynamics can develop very slow and very fast time scales separated by a range of active time scales.

The G-Scheme is a time accurate explicit solver that exploits all opportunities for on-line reduction of stiff systems, which arise when the gaps in the fast/active and slow/active time scales become sufficiently large. We provided an asymptotic analysis and proposed a numerical technique consisting of an algorithmic framework in [13], to achieve multi-scale adaptive model reduction along-with the integration of non-stiff ordinary differential equations (ODEs) using objective criteria. In the G-Scheme, it is assumed that the dynamics is (locally) decomposed into active, slow, fast, and when applicable, invariant subspaces. The method is directly applicable to initial-value ODEs and (by using the method of lines) to partial differential equations (PDEs). Below, we give a brief overview of the method. The interested reader is referred to [13] for details and extensive discussions regarding the method, its accuracy, computational cost, and illustrative application examples.

Consider the Cauchy problem defined by a set of autonomous ODEs:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}(t)), \qquad \mathbf{x}(t_0) = \mathbf{x}_0, \tag{1}$$

with time $t \in (t_0, t_f] \subset \mathbb{R}$, the state vector $\mathbf{x} \in \mathbb{R}^N$, and the nonlinear vector field $\mathbf{f} : E \subset \mathbb{R}^N \Rightarrow \mathbb{R}^N$. The component-wise representation of the perturbation vector $\Delta\mathbf{x}(t)$ can be expressed in terms of curvilinear coordinates $\Delta\mathbf{x} = \Delta\xi^i \mathbf{a}_i = \Delta\xi_j \mathbf{b}^j$ related to the sets of covariant and contravariant basis vectors $\mathbf{a}_i$ and $\mathbf{b}^j$, having the properties $\mathbf{a}_i \cdot \mathbf{b}^j = \delta_i^j$. The G-Scheme identifies the set of basis vectors $\mathbf{a}_i$ with the right eigenvectors of the Jacobian matrix J of the vector field, and the dual vectors $\mathbf{b}^j$ coinciding with the left eigenvectors of J. In the case of a homogenous reactive system the vector field $\mathbf{f}(\mathbf{x})$ can be expressed as

$$\mathbf{f}(\mathbf{x}) = \mathbf{S}_k r^k(\mathbf{x}) = \mathbf{a}_i(\mathbf{x}) g^i(\mathbf{x}), \tag{2}$$

where $\mathbf{S}_k$ and r^k are the stoichiometric vector and the rate associated with the kth reaction, and k ranges from 1 to the number of reversible reactions, N_r. The scalar g^i is defined as

$$g^i(\mathbf{x}) = \mathbf{b}^i(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = \mathbf{b}^i(\mathbf{x}) \cdot \mathbf{S}_k r^k(\mathbf{x}). \tag{3}$$

The amplitude and direction of the ith mode are g^i and $\mathbf{a}_i$, respectively. Note that g^i provides the contribution of the ith mode to the vector field $\mathbf{f}(\mathbf{x})$ since each basis vector $\mathbf{a}_i$ is normalized to have unit norm.

The ordering of the basis vectors is fundamental for a proper decomposition into active, slow, fast, and invariant subspaces. In the G-Scheme, the basis vectors $\mathbf{a}_j$ are ranked according to the magnitude of the modulus of the (possibly complex) eigenvalues, λ_j:

$$\begin{aligned} 0 = \lambda_1 = \cdots = \lambda_E < |\lambda_{E+1}| \le \cdots \le |\lambda_{H-1}| \ll |\lambda_H| \le \cdots \\ \cdots \le |\lambda_T| \ll |\lambda_{T+1}| \le \cdots \le |\lambda_N|, \end{aligned} \tag{4}$$

where $0 = \lambda_1 = \cdots = \lambda_E$, $|\lambda_{E+1}| \le \cdots \le |\lambda_{H-1}|$, $|\lambda_H| \le \cdots \le |\lambda_T|$, and $|\lambda_{T+1}| \le \cdots \le |\lambda_N|$, identify the time scales in the invariant, $\mathbb{E}$, slow, $\mathbb{H}$, active, $\mathbb{A}$, and fast, $\mathbb{T}$, subspaces, respectively. The decomposition induced by the above time scale ordering assumes that the tangent space $\mathcal{T}_x$ is given by the direct sum of the four subspaces:

$$\mathcal{T}_x = \mathbb{E} \oplus \mathbb{H} \oplus \mathbb{A} \oplus \mathbb{T}, \tag{5}$$

where the active subspace $\mathbb{A}$ contains all the intermediate, currently active (dynamic) time scales, all scales slower/faster than the active ones are confined in the subspaces $\mathbb{H}/\mathbb{T}$, and, if the system possesses E invariants, $\mathbb{E}$ is the subspace spanned by the directions associated with them. With the above definitions, $N_E = \dim(\mathbb{E}) = E$, $N_H = \dim(\mathbb{H}) = H - E - 1$, $N_A = \dim(\mathbb{A}) = T - H + 1$, and $N_T = \dim(\mathbb{T}) = N - T$. Note that, because of this ordering, (possibly complex) eigenvalues with both negative and positive real parts can be found in $\mathbb{H}$ and $\mathbb{A}$, whereas we expect the eigenvalues in $\mathbb{T}$ to have dominant negative real parts. Indeed, this is the distinguishing feature of the class of problems for which the G-Scheme is expected to perform most effectively. The ratio ϵ_H is a measure of the spectral gap between the slow and active subspaces, while ϵ_T is a measure of the spectral gap between the active and fast subspaces, and they are defined as:

$$\epsilon_H \equiv \frac{|\lambda_{H-1}|}{|\lambda_H|} \ll 1, \qquad \epsilon_T \equiv \frac{|\lambda_T|}{|\lambda_{T+1}|} \ll 1, \tag{6}$$