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Coupling of the model reduction technique with the lattice Boltzmann method for combustion simulations

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ABSTRACT

A new framework of simulation of reactive flows is proposed based on a coupling between accurate reduced reaction mechanism and the lattice Boltzmann representation of the flow phenomena. The model reduction is developed in the setting of slow invariant manifold construction, and the simplest lattice Boltzmann equation is used in order to work out the procedure of coupling of the reduced model with the flow solver. Practical details of constructing slow invariant manifolds of a reaction system under various thermodynamic conditions are reported. The proposed method is validated with the two-dimensional simulation of a premixed counterflow flame in the hydrogen-air mixture.

1. Introduction

Accurate modeling of reactive flows requires the solution of a large number of conservation equations as dictated by detailed reaction mechanism. In addition to the sometimes prohibitively large number of variables introduced, the numerical solution of the governing equations has to face the stiffness due to disparate time scales of the kinetic terms. These issues make computations of even simple flames time consuming, and have particularly negative impact on the lattice Boltzmann method [31,32], whose number of fields (distribution functions or populations) may be significantly larger than the number of conventional fields (density, momenta, temperature, species mass fractions). The lattice Boltzmann (LB) method is a relatively novel approach to numerical flow simulations, and recent studies have proved that it is competitive to traditional methods when simulating compressible [28] and turbulent flows [29] in terms of both accuracy and efficiency. Although this makes LB a good candidate for computing reactive flows, applications in this field are still limited by the stiffness of the governing equations and the large number of fields to solve.

On the other hand, the difference of time scales can be exploited in order to construct a reduced description of the detailed model. In fact, because of the stiffness, the dynamics of homogeneous reactive systems is often characterized by a short transient towards a low dimensional manifold in the concentration space, known as the *slow invariant manifold* (SIM). The subsequent dynamics is slower and it proceeds along the manifold itself, until a steady state is reached. Constructing such manifolds can lead to a simpler and less stiff description of the reactive system, where the fast transient is neglected and the slow dynamics can be reproduced with high accuracy. Therefore, much effort has been devoted to achieving that aim; the intrinsic low dimensional manifold (ILDM) approach [35], the computational singular perturbation (CSP) method [36] and the Flamelet-Generated Manifolds (FGM) method [22,23] are representative examples.

In this work, we make use of the method of invariant grids (MIG) [1–3] which is also based on the notion of SIM, and it has been recently elaborated for combustion applications [8,9] with the aim of automating the model reduction procedure. In particular, its realization follows two key steps. First, an initial rough reduced description of the complex chemical mechanism is constructed making use of the notion of *quasi equilibrium manifold* (QEM). Second, the latter initial approximation is iteratively refined until the *invariant grid* is constructed. Finally, we employ the reduced model of the hydrogen mechanism in a lattice Boltzmann code for simulating laminar flames throughout a homogeneous mixture.

This paper is organized in sections as follows. In Section 2, the kinetic equation for a batch reactor is reviewed. The construction of a reduced model using the method of invariant grids is briefly

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described in Section 3. In Section 4, the lattice Boltzmann method for reactive flows is reviewed, and the coupling with a reduced model is presented in Section 4.2. Results are discussed in Section 5. A detailed discussion on the construction of thermodynamic Lyapunov functions, and on the exact computation of their derivatives (as requested in order to implement the MIG to combustion applications) is presented in Appendix A. Finally, the exact evaluation of the Jacobian matrix of a system of kinetic equations is addressed in the Appendix B.

2. Detailed reaction kinetics in a batch reactor

In this section, we focus on homogeneous mixtures of ideal gases reacting in a closed system. Let $x_1,\ldots,x_n$ be n chemical species participating in a detailed reaction mechanism with r reversible steps

$$v'_{s1}x_1 + \cdots + v'_{sn}x_n \rightleftharpoons v''_{s1}x_1 + \cdots + v''_{sn}x_n, \quad s = 1,\ldots,r, \tag{1}$$

where v'_{si} and v''_{si} are the stoichiometric coefficients of species i in the reaction step s for reactants and products. Let the stoichiometric vectors be $\boldsymbol{v}'_s = (v'_{s1},\ldots,v'_{sn})$, $\boldsymbol{v}''_s = (v''_{s1},\ldots,v''_{sn})$ and $\boldsymbol{v}_s = \boldsymbol{v}''_s - \boldsymbol{v}'_s$. The reaction rate of step s reads

$$\begin{aligned} &\Omega_s = \Omega_s^+ - \Omega_s^-, \\ &\Omega_s^+ = k_s^+(T)\prod_{i=1}^{n} c_i^{\alpha_i}, \quad \Omega_s^- = k_s^-(T)\prod_{i=1}^{n} c_i^{\beta_i}. \end{aligned} \tag{2}$$

Let N_i and V be the mole number of species i and the reactor volume, respectively, the corresponding molar concentration is given by $c_i = N_i/V$. The forward and reverse reaction rate constants k_s^+, k_s^- take the Arrhenius form

$$k_s(T) = A_s T^{\beta_s} \exp\left(\frac{-E_{as}}{\mathscr{R}T}\right), \tag{3}$$

where A_s denotes the pre-exponential factor, β_s the temperature exponent, E_{as} the activation energy of reaction s and $\mathscr{R}$ is the universal gas constant. The rate of change of species i is given by

$$\dot{\omega}_i = \sum_{s=1}^{r} \boldsymbol{v}_s(i)\Omega_s, \quad i = 1,\ldots,n, \tag{4}$$

with forward and reverse reaction rate constants related by the equilibrium constant $K_{c,s} = k_s^+/k_s^-$, which can be obtained by imposing the *principle of detail balance* at the steady state:

$$\Omega_s^+ = \Omega_s^-, \quad s = 1,\ldots,r. \tag{5}$$

In the following, an arbitrary point of the composition space will be denoted by $\boldsymbol{c} = (c_1,\ldots,c_n)$, where c_i is the molar concentration of species i. Moreover, a given state of a homogeneous ideal gas mixture is fully described by a vector $\boldsymbol{c}$ and one independent *intensive* property, e.g., the corresponding temperature T. An alternative description of the system is also given by $\boldsymbol{\psi} = (Y_1,\ldots,Y_n)$ and two independent intensive properties, e.g., temperature T and total pressure p, where Y_i is the mass fraction of species i.

Under isochoric and isothermal conditions (V, $T = const$), the reaction kinetic Eq. (4) are closed, and the temporal evolution of the species concentrations in the reactor obeys the following system of ordinary differential equations:

$$\frac{d\boldsymbol{c}}{dt} = (\dot{\omega}_1,\ldots,\dot{\omega}_n)^T = \boldsymbol{f}, \tag{6}$$

whereas, for different cases, additional closure relations are needed. Two cases are relevant to combustion: isolated reactor with constant volume and mixture-averaged internal energy ($V, \overline{U} = const$), and thermal isolated isobaric reactor with constant total pressure and mixture-averaged enthalpy ($p, \bar{h} = const$). In the first case, the governing equations read

$$\begin{aligned} &\overline{U} = \sum_{i=1}^{n} U_i(T)Y_i = const, \\ &\frac{d\boldsymbol{c}}{dt} = (\dot{\omega}_1,\ldots,\dot{\omega}_n)^T = \boldsymbol{f}, \end{aligned} \tag{7}$$

where for each species i, the temperature dependence of the specific internal energy U_i is taken into account by a polynomial fit

$$U_i(T) = \mathscr{R}\left(a_{1i}T + \frac{a_{2i}}{2}T^2 + \frac{a_{3i}}{3}T^3 + \frac{a_{4i}}{4}T^4 + \frac{a_{5i}}{5}T^5 + a_{6i}\right) - \mathscr{R}T. \tag{8}$$

Here, following [42], the temperature dependence of thermodynamic properties of species i are expressed in terms of tabulated constants a_{ji}, with $j = 1,\ldots,7$.

Let W_i be the molecular weight of species i, for closed reactors under fixed total pressure and mixture-averaged enthalpy, the dynamics of the mass fractions Y_i obeys the following equation system

$$\begin{aligned} &\bar{h} = \sum_{i=1}^{n} h_i(T)Y_i = const, \\ &c_i = \frac{p(Y_i/W_i)}{\mathscr{R}T\sum_{j=1}^{n} Y_j/W_j}, \\ &\frac{d\boldsymbol{\psi}}{dt} = \left(\frac{W_1\dot{\omega}_1}{\bar{\rho}},\ldots,\frac{W_n\dot{\omega}_n}{\bar{\rho}}\right)^T = \boldsymbol{f}, \end{aligned} \tag{9}$$

where the mixture density $\bar{\rho}$ and the specific enthalpy h_i of species i take the explicit form

$$\bar{\rho} = \sum_{i=1}^{n} W_i c_i, \quad h_i(T) = U_i(T) + \mathscr{R}T. \tag{10}$$

Notice that, for non-isothermal cases, the temperature corresponding to the composition state $\boldsymbol{\psi}$ is not explicitly known. Therefore, the right-hand side of (4) can be evaluated after solving the two energy conservation equations in (7) and (9) with respect to T (e.g., using the Newton–Raphson method).

Finally, in a closed chemically reactive system, the atom mole numbers N_k of each element k must be conserved:

$$\boldsymbol{D}\boldsymbol{\psi}^T = (N_1,\ldots,N_d)^T, \quad \frac{dN_k}{dt} = 0, \quad \boldsymbol{D}(k,i) = \frac{\mu_{ik}}{W_i}, \tag{11}$$

where μ_{ik} is the number of atoms of the kth element in species i, and $\boldsymbol{D}$ is a $(d \times n)$ matrix, while d is the number of elements involved in the reaction. In other words, the vector field $\boldsymbol{f}$ of motions in the phase-space is always orthogonal (in Euclidean sense) to the rows of $\boldsymbol{D}$.

The interested reader is delegated to the classical work of Williams [40] for a detailed discussion on the theory of chemical kinetics.

3. Reduced description

In our study, the detailed mechanism of Li et al. [4] (9 species, 21 elementary reactions) for hydrogen combustion is considered, and we search for a reduced description with two degrees of freedom. Here, we present a general overview of the method of invariant grids (MIG) for model reduction in chemical kinetics. The interested reader can find more details in Refs. [1,2,6–9].

3.1. Initial approximation: quasi equilibrium manifold

Approximated reduced descriptions in chemical kinetics can be based on the notion of quasi equilibrium manifold [1,2]. Hence, let us construct a quasi equilibrium manifold for a stoichiometric H_2-air mixture under fixed pressure $p = 1$ bar and enthalpy $\bar{h} = 2.8$ kJ/kg, corresponding to the temperature $T_0 = 300$ K for the stoichiometric unburned mixture $H_2 + 0.5O_2 + 1.88N_2$. A generic $q -$ dimensional QEM is obtained by solving the following minimization problem: