Invariant Grids and Lattice Boltzmann Method for Combustion

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***Abstract*— The lattice Boltzmann (LB) method is a relatively novel approach to numerical flow simulations, and recent studies have proved that it is highly competitive to traditional methods when simulating compressible and turbulent flows (in terms of 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 amount of fields to solve. In this sense, the present study intends to provide an effective tool for reactive flow simulations via the LB method.**

I. 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 the fast 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, whose number of fields (distribution functions or populations) is significantly larger than the number of conventional fields (density, momenta, temperature, species mass fractions) by a factor ranging from tens to hundreds for 2D and 3D simulations. However, the dynamics of complex reactive systems is often characterized by short initial transients when the solution trajectories approach low-dimensional manifolds in the concentration space, known as the *slow invariant manifolds* (SIM). Thus, the construction of SIM enables to establish a simplified description of a complex system by extracting only the slow dynamics and neglecting the fast.

The Method of Invariant Grids (MIG), based on the concept of SIM, has been elaborated for combustion applications with the aim of automating the model reduction procedure, and 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. In fact, according to MIG, the accurate reduced model (invariant grid) is the stable fixed point of one of the following processes: Newton-like iterations for solving the *invariance condition* regarded as an equations, or relaxation due to a *film equation* of dynamics [1], [2]. Lately, the reduced model of the hydrogen mechanism can be employed in a lattice Boltzmann code for simulating laminar flames throughout a homogeneous mixture.

II. REDUCED DESCRIPTION

In our study, the detailed mechanism of Li et al [3] (9 species, 21 elementary reactions) for hydrogen combustion is considered, and we search for a reduced description with two degrees of freedom. To this end, let us construct the $2D$ quasi equilibrium manifold for a stoichiometric H_2-air mixture under fixed pressure $p = 1bar$ and enthalpy $\bar{h} = 2.8kJ/kg$, corresponding to the temperature $T_0 = 300K$ for the stoichiometric unburned mixture $H_2+0.5O_2+1.88N_2$. A QEM is obtained solving the following minimization problem:

$$\begin{array}{ll} min & G \\ s.t. & \sum\limits_i m_j^i Y_i = \xi^j, \quad j = 1, 2. \end{array} \tag{1}$$

Here, G represents the mixture-averaged entropy, and the vector set $\{\boldsymbol{m}_j = (m_j^1, ..., m_j^9)\}$ is used to reparameterize the mass fractions Y_i in terms of new variables ξ^j, which are expected to follow a slow dynamics. Many suggestions for defining slow lumped variables in chemical kinetics are known in the literature, and for our purposes here we use the *total number of moles* ξ^1 and *free oxygen* ξ^2, respectively (see, e.g., [4]). An approximated solution to (1), computed making use of the algorithm introduced in [5], is shown in Fig. 1, and it is called *quasi equilibrium grid* (QEG). The corresponding invariant grid is found by relaxation of the QEG Ω under the following film equation of dynamics [1]

$$\frac{d\Omega}{dt} = \vec{f} - \boldsymbol{P}\vec{f}, \tag{2}$$

where $\vec{f}$ and $\boldsymbol{P}$ denote the vector of motion in the phase space and a projector operator onto the manifold tangent space, respectively. Following [1], here we adopt the *thermodynamic projector* which enables to define the fast motions toward the slow manifolds. Finally, the refined grid, approximating the slow invariant manifold, is shown in Fig. 2. More details can be found in the literature [6], [7], [8].

III. LATTICE BOLTZMANN FOR REACTIVE FLOWS

We consider here the simplest lattice Boltzmann formulation suitable for simulations of combustion. To this

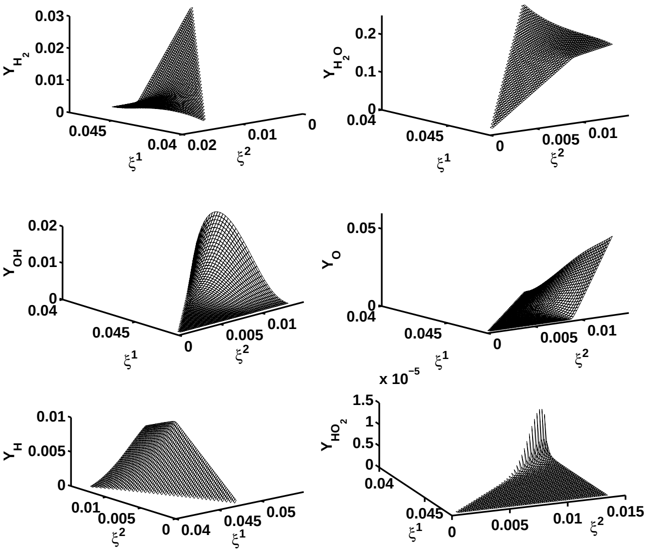

Fig. 1. Quasi equilibrium grid (QEG): Six coordinates function of the parameters ξ^1, ξ^2.

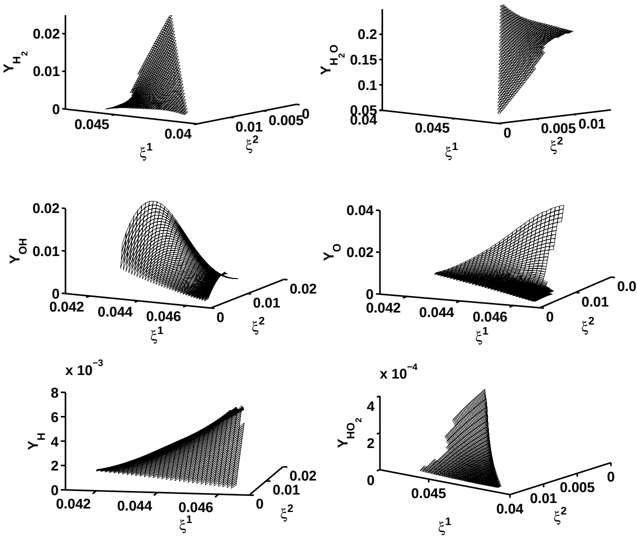

Fig. 2. Invariant grid approximating the slow invariant manifold.

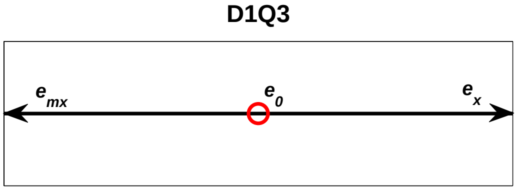

Fig. 3. 1-dimensional 3-velocities lattice: $D1Q3$.

end, following the suggestion of Yamamoto et al [9], reactive flows can be simulated with the lattice Boltzmann method as reported below. Note, however, that more elaborate and complete LB models for mixtures [10], [11] and compressible flows [12] shall be taken into account in the near future, too. According to the standard terminology, LB schemes are denoted as DMQN, meaning that N particles move on a M-dimensional lattice. In Fig. 3, the most popular one-dimensional lattice is shown, where each distribution function is represented by its own peculiar velocity $\boldsymbol{e}_\alpha$. In the following, we briefly review the LB algorithm with the BGK [13] collision model. A single-component medium is described by a small set of populations, which can be regarded as microscopic properties of the fluid. On the contrary, macroscopic quantities such as density and momentum (energy for thermal cases) are given by different moments of those populations. In terms of pressure distribution functions p_α, the LB equation takes the following discrete form at the lattice node $\boldsymbol{x}$:

$$\begin{gathered} p_\alpha\left(\boldsymbol{x}+\boldsymbol{e}_\alpha, t+\delta t\right) = p_\alpha\left(\boldsymbol{x}, t\right) - \\ \frac{1}{\tau_F}\left[p_\alpha\left(\boldsymbol{x}, t\right) - p_\alpha^{eq}\left(p, \boldsymbol{u}\right)\right], \end{gathered} \tag{3}$$

where the equilibrium populations p_α^{eq} read:

$$p_\alpha^{eq} = w_\alpha p\left[1 + 3\left(\boldsymbol{e}_\alpha \boldsymbol{u}^T\right) + \frac{9}{2}\left(\boldsymbol{e}_\alpha \boldsymbol{u}^T\right)^2 - \frac{3}{2}\boldsymbol{u}^2\right]. \tag{4}$$

The pressure p and the fluid velocity $\boldsymbol{u}$ are given by:

$$p = \sum_\alpha p_\alpha, \quad \boldsymbol{u} = \frac{1}{p_0}\sum_\alpha \boldsymbol{e}_\alpha p_\alpha, \tag{5}$$

where the reference pressure $p_0 = \rho_0/3$, with ρ_0 denoting the reference density of the LB model. Let δt be the time step, the relaxation parameter τ_F is related to the kinematic viscosity ν by (see, e.g., [14])

$$\nu = \frac{2\tau_F - 1}{6}\delta t. \tag{6}$$

In general, the discrete velocities can be regarded as the nodes of a Gauss-Hermite quadrature applied to the Maxwell- Boltzmann distribution function, and each of them is characterized by a proper weight w_α.

According to [9], the flow field is not affected by the chemical reaction, transport coefficients are constant and Fick's law applies to the diffusion. In this case, the background flow is treated as an one-component medium whose pressure populations evolution obeys (3). Let $\bar{h}_0$ be a reference enthalpy, the evolution equations for enthalpy and concentration of species i are written as

$$\begin{gathered} \tilde{h}_\alpha\left(\boldsymbol{x}+\boldsymbol{e}_\alpha, t+\delta t\right) - \tilde{h}_\alpha\left(\boldsymbol{x}, t\right) = \\ -\frac{1}{\tau_h}\left[\tilde{h}_\alpha\left(\boldsymbol{x}, t\right) - \tilde{h}_\alpha^{eq}\left(\tilde{h}, \boldsymbol{u}\right)\right] + w_\alpha Q_h, \end{gathered} \tag{7}$$

$$\begin{gathered} Y_{i\alpha}\left(\boldsymbol{x}+\boldsymbol{e}_\alpha, t+\delta t\right) - Y_{i\alpha}\left(\boldsymbol{x}, t\right) = \\ -\frac{1}{\tau_{Y_i}}\left[Y_{i\alpha}\left(\boldsymbol{x}, t\right) - Y_{i\alpha}^{eq}\left(Y_i, \boldsymbol{u}\right)\right] + w_\alpha Q_{Y_i}, \end{gathered} \tag{8}$$

where

$$\tilde{h} = \bar{h}/\bar{h}_0 = \sum_\alpha \tilde{h}_\alpha, \quad Y_i = \sum_\alpha Y_{i\alpha}, \tag{9}$$

and the equilibrium populations $\tilde{h}_\alpha^{eq}$, $Y_{i\alpha}^{eq}$ are expressed as in (4) after replacing p with $\tilde{h}$ and Y_i, respectively. Assume t_0 is a factor for converting physical time into LB time units: $(t)_{LB} = (t)_{phys}\big/t_0$, the source terms take the explicit form

$$Q_h = \frac{1}{\bar{h}_0}\left(\sum_{i=1}^{9}\frac{\dot{\omega}_i W_i}{\bar{\rho}}h_i\right)t_0\delta t, \; Q_{Y_i} = \frac{\dot{\omega}_i W_i}{\bar{\rho}}t_0\delta t, \tag{10}$$

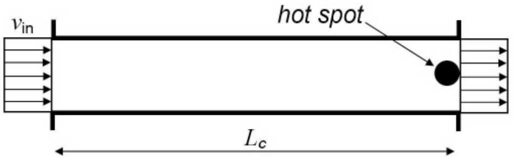

Fig. 4. Schematic representation of the $1D$ setup.

where $\bar{\rho}$ is the mixture-averaged density, while $\dot{\omega}_i$, W_i, h_i denote the rate of change, molecular weight and enthalpy of species i, respectively. The thermal diffusivity κ and diffusion coefficient D_i of species i are related to the relaxation parameters as follows [14]

$$\kappa = \frac{2\tau_h - 1}{6}\delta t, \quad D_i = \frac{2\tau_{Y_i} - 1}{6}\delta t. \tag{11}$$

IV. EXAMPLE: FREELY PROPAGATING FLAME

In the following, we consider a stoichiometric hydrogen-air mixture entering an adiabatic channel (constant cross section) under room conditions ($T = 300K$, $p = 1bar$) at fixed velocity $v_{in} = 1.2m/s$. A heat source is placed at the outlet in order to ignite the mixture (see Fig. 4). A flame front is formed and propagates upstream since the laminar flame speed is larger than the flow velocity.

For simplicity, we use the assumption of equal diffusivity D for all species and Lewis number $Le = \kappa/D = 1$. In this case, the mixture enthalpy $\bar{h}$ and the element fractions remain constant throughout the domain, and the reduced dynamics takes place along the invariant grid constructed as discussed in the section II. Notice however that, the latter assumption is not restricting and a generalization is obtained by extending the invariant grid with enthalpy and element fractions as additional degrees of freedom. On the other hand, in premixed systems, those quantities are conserved up to small fluctuations and, for such applications, the invariant grid is often sufficient. Finally, in low-Mach combustion, the pressure p can be considered constant for most cases.

Under the latter assumptions, the equations (8) can be written in terms of the slow manifold parameters ξ^1, ξ^2 as follows:

$$\begin{split} \xi^j_\alpha\left(\boldsymbol{x} + \boldsymbol{e}_\alpha, t + \delta t\right) - \xi^j_\alpha\left(\boldsymbol{x}, t\right) = \\ -\frac{1}{\tau_\xi}\left[\xi^j_\alpha(\boldsymbol{x}, t) - \xi^{jeq}_\alpha\left(\xi^j, \boldsymbol{u}\right)\right] + w_\alpha Q_{\xi^j}, \end{split} \tag{12}$$

where, the equilibrium populations for the reduced variables ξ^j read

$$\xi^{jeq}_\alpha = w_\alpha \xi^j \left[1 + 3\left(\boldsymbol{e}_\alpha \boldsymbol{u}^T\right) + \frac{9}{2}\left(\boldsymbol{e}_\alpha \boldsymbol{u}^T\right)^2 - \frac{3}{2}\boldsymbol{u}^2\right], \tag{13}$$

and the source terms take the form:

$$Q_{\xi^j} = \sum_{i=1}^{9} m^i_j Q_{Y_i}, \; \xi^j = \sum_{i=1}^{9} m^i_j Y_i. \tag{14}$$

The setup of Fig. 4 was simulated by solving both the detailed model (7), (8) and the reduced one (12). In the latter case, the source terms Q_{ξ^j} are tabulated at each node of the invariant grid, and accessed through multivariate linear interpolation. When simulating the reduced model, a remarkable saving, in terms of both memory (one-quarter of the density functions are stored at any lattice node) and number of time steps ($\delta t_{reduced} \cong 35\delta t_{detailed}$), can be achieved. Moreover, based on the comparison in Fig. 5, we can argue that the suggested methodology enables to perform detailed simulations with high accuracy. Finally, in Fig. 6 the flame position is shown as function of time. The flame is defined as the point with the highest heat release Q_h at a given time. The linear dependence indicates that the flame moves at constant speed given by: $S_L = \text{slope} + v_{in} \cong 2.26m/s$. The value of the burning velocity S_L is in perfect accordance with the detailed model prediction (up to 2%) and in a good agreement with experimental data (see, e.g. [15]).

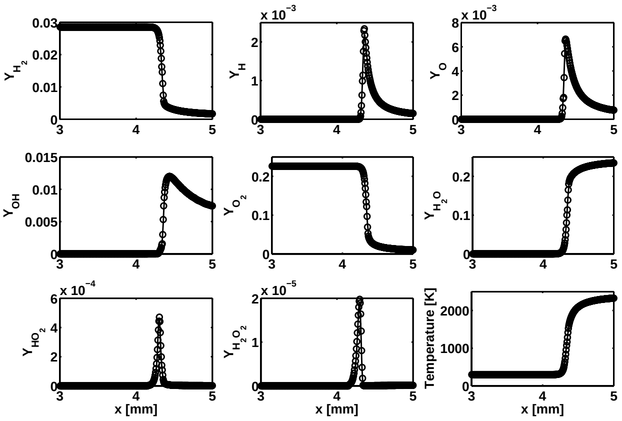

Fig. 5. Fields along the channel at a given time: detailed model (continuous line) and reduced model (circles).

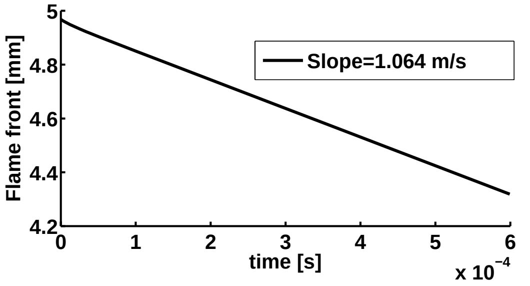

Fig. 6. Flame front position vs time with the inlet velocity $v_{in} = 1.2m/s$.

V. EXAMPLE: PREMIX COUNTERFLOW FLAMES

Here, we consider the so-called counterflow laminar flame as a two dimensional benchmark of the suggested methodology. A well premixed stoichiometric H_2-air mixture is uniformly ejected from two parallel stationary flat nozzles, located at $y = \pm L_y$. When properly ignited, the fuel reacts generating two twin flames in this counterflow, while the burned gas exits the domain along the x-direction. As illustrated in the sketch of Fig. 7, under the assumption of symmetrical flow with respect to the stagnation lines $x = 0$ and $y = 0$, the computational

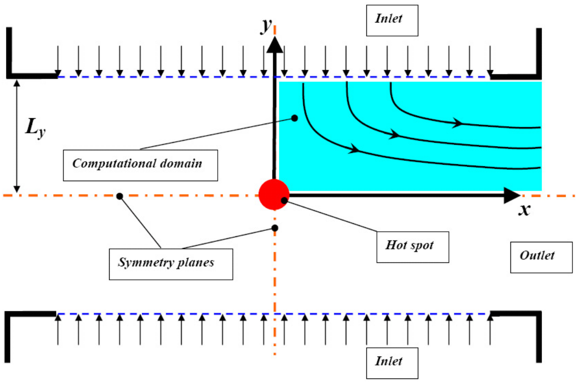

Fig. 7. Schematic representation of the 2D setup.

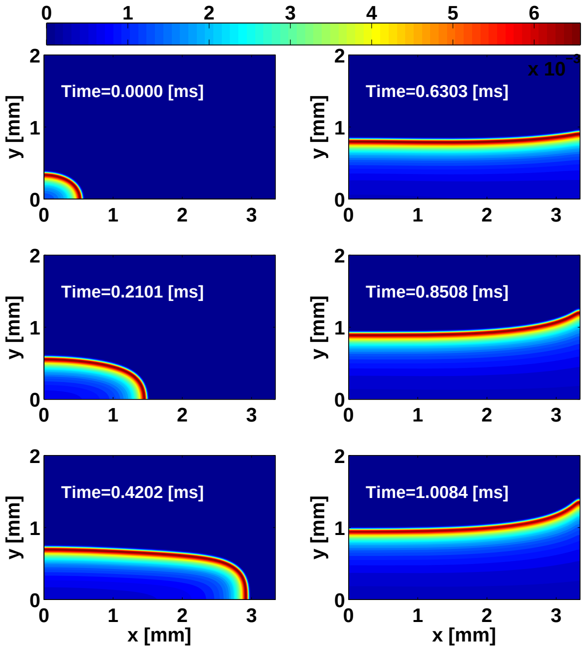

Fig. 8. Detailed model using the $D2Q9$ lattice: O mass fraction evolution

domain can be restricted to the region where $x \geq 0$ and $y \geq 0$, and simulations can be carried out using the standard 2-dimensional lattice $D2Q9$. In both models (detailed and reduced), the mixture, initially under room temperature $T_0 = 300K$, is ignited by placing a hot spot at the origin of the reference system. Very good agreement is demonstrated as reported in Figures 8 and 9, where the time evolution of O radical concentration is shown.

VI. CONCLUSIONS

Here, we suggest a methodology for using accurate reduced chemical kinetics in combination with a lattice Boltzmann solver for simulating reactive flows. It has been shown that the Method of Invariant Grids (MIG) is suitable for providing the reduced description of chemistry, and this approach enables to cope with stiffness when solving the LB species equations. This is particularly desirable in the case of explicit solvers, and it results in a remarkable speedup.

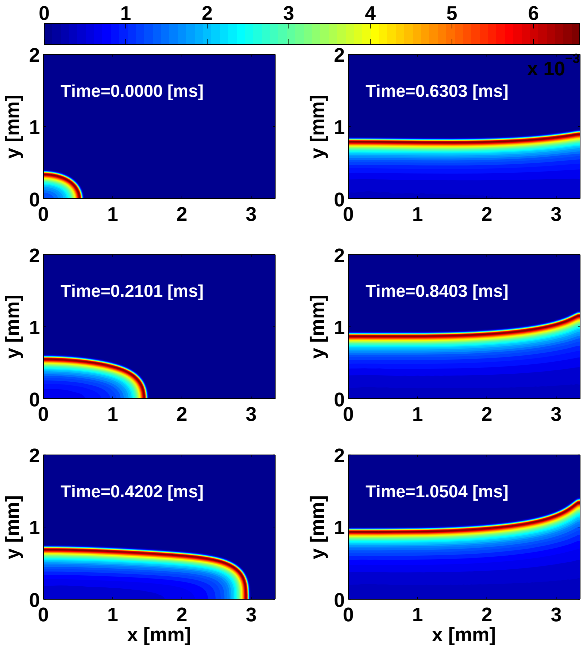

Fig. 9. Reduced model using the $D2Q9$ lattice: O mass fraction evolution

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