A Combined Adaptive Chemistry and Tabulation Strategy for the Efficient Implementation of Detailed Combustion Chemistry

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***Abstract*— Significant progress is being made in the development of detailed chemical kinetic mechanisms for transportation fuels and their surrogates, leading to models involving up to several thousands molecular species. A major challenge is to make use of this chemical knowledge in turbulent combustion models, which most often become intractable if more than tens of species are considered. In this work, we propose a novel adaptive chemistry strategy specifically designed for LES/particle PDF simulations of non-premixed turbulent flames with the following key properties: (i) the composition space is partitioned *a priori* into a user-specified number of regions, over which suitable reduced chemical representations and chemical models are identified; (ii) the computational particles in the LES/PDF simulations carry only the variables present in the reduced representations; and (iii) the region a given particle belongs to is identified using a low-dimensional binary tree search algorithm, thereby keeping the run-time overhead associated with the adaptive approach to a minimum. An overview of the adaptive strategy is first presented, with details being provided for the major components of the algorithm. The adaptive treatment of the chemistry is then implemented within the ISAT/RCCE framework validated previously by Hiremath *et al.* [Hiremath, Ren & Pope, Combust. Flame, 2011]. A proof-of-concept of the combined adaptive chemistry and tabulation strategy is presented for the simpler partially stirred reactor (PaSR) with pair-wise mixing configuration. Preliminary results indicate that compared to results based on a single reduced representation for all particles, the adaptive methodology provides similar accuracy at a lower overall computational cost.**

I. Introduction

The understanding of chemical kinetics for hydrocarbon fuel combustion has exploded over the past two decades, leading to the development of ever growing detailed kinetic schemes for a wide range of molecular species relevant to hydrocarbon combustion [1]. With more accurate rate rules and improved mechanistic considerations, some of the latest published mechanisms are approaching 10^4 species and as many reactions [2]. However, these advances in chemical kinetics and detailed model development have to be integrated with Computational Fluid Dynamics (CFD) tools to fully realize their potential in terms of improved understanding and optimization of practical combustion devices. The real challenge then is to maximize the level of chemical detail that can be afforded in CFD. One strategy to address this challenge was recently proposed by Hiremath *et al.* using a combination of dimension reduction and tabulation [3] and applied to the simulation of turbulent flames. Such techniques greatly increase the level of description of the chemistry that can be used, allowing, for example, the use of about 40 species in large-eddy simulation/probability density function (LES/PDF) calculations. However, significant further gains are clearly needed to handle the chemical complexities of real fuels, which can be attained through the development of adaptive chemistry methodologies, in which (ideally), in different regions of the flow, the smallest possible reduced mechanism is used as required by the local chemical activity and thermodynamic state. Several adaptive chemistry approaches have been proposed recently in the literature (*e.g.* [4], [5], [6], [7], [8], [9]), generally yielding quite promising results.

In this work, we propose an adaptive strategy to handle large chemical mechanisms tailored for LES/PDF simulations of non-premixed combustion, with the following constraints: the framework should be compatible and work synergistically with existing LES/PDF implementations (*e.g.*[10]), the overhead cost associated with the adaptive treatment of the chemistry should be small, and only reduced representations should be used to evolve the composition of the particles. In the following, a overview of the adaptive methodology is provided, and the integration of the adaptive algorithm within the ISAT/RCCE framework of Hiremath *et al.* [3] is discussed.

II. Adaptive Chemistry Methodology

We consider a detailed chemical mechanism involving a set of species $\mathbf{\Phi}^D$, of cardinality n_D, and we denote the mass fraction of the species by the n_D-vector $\mathbf{Y}$. We consider the case of constant-pressure combustion, so that the thermochemical state of the fluid is fully characterized by $\mathbf{Y}$ and the temperature T. In the LES/PDF calculation, the fluid within the turbulent flow field is represented by a large number of particles. At time t, the nth particle has a composition $\mathbf{C}^{(n)}(t) = \{\mathbf{Y}^{(n)}(t), T^{(n)}(t)\}$. The simulation

marches in time in uniform time steps Δt. While the particles move in physical space due to the resolved flow and the unresolved turbulence, the particle compositions change due to just two processes: reaction and mixing. We call reaction mapping over a time step Δt the evolution from $\mathbf{C}^{(n)}(t)$ to $\mathbf{C}^{(n)}(t+\Delta t)$ due to reaction. In this context, our approach to adaptive chemistry is decomposed into a pre-processing step to define the reduced chemistry framework *prior to* the flame simulations, and a procedure to dynamically assign the appropriate reduced representation and model to each of the particles *during* the flame simulation. More specifically, the strategy consists of the following components:

A. Pre-processing of the chemical kinetics

The pre-processing uses the detailed kinetic model in simpler Partially Stirred Reactor calculations, whose conditions are representative of the turbulent flame simulation to be performed, to generate a large database of detailed test compositions. This database is used for:

1) **Partitioning:** Suitably partition the composition space into a number of regions, the J^{th} one being denoted by R_J, using a cutting-plane method.
2) **Reduction:** For each region R_J, develop an accurate reduced chemical model M_J, in which the composition has a reduced representation $\mathbf{c}_J = \{\mathbf{y}_J, T_J\}$. The reduced mass fraction vector $\mathbf{y}_J$ is of size $n_{R,J} \ll n_D$. This is accomplished using the Directed Relation Graph with Error Propagation reduction technique [11].

The partition then is stored as a binary tree, associated with a set of reduced models, one for each leaf of the tree, and a set of cutting planes, one for each node of the tree.

B. Adaptive approach in flame simulation

In the LES/PDF computations, the particle composition located in region R_J carries the reduced composition $\mathbf{c}_J^{(n)}(t) = \{\mathbf{y}_J^{(n)}(t), T_J\}$ instead of $\mathbf{C}^{(n)}(t)$, and this composition is advanced during the reaction sub-step using the reduced model M_J. This requires two main procedures:

1) **Conversion:** Convert a particle composition from reduced representation J to reduced representation L as the particle moves across regions. A simple merge of the representations, followed by normalization is used here to get the new mass fraction vector.
2) **Classification:** An efficient binary tree search based on a well-chosen small set of species is used to determine the region a given particle belongs to based on its reduced representation.

III. Preliminary Results

The adaptive strategy is tested using PaSR calculations for non-premixed propane/air and a detailed mechanism containing 115 species [12]. The composition space is partitioned into 20 regions based on a detailed sample database of 10^4 compositions. The evolution of the particle compositions are then compared to the detailed solution for different levels of reductions, and shown in Fig. 1. The errors obtained when using a single reduced representation and single reduced model for all particles are also shown. While only basic algorithms for all components involved in the adaptive approach have been implemented, these results indicate that the adaptive methodology provides similar accuracy at a lower overall computational cost compared to single model approaches.

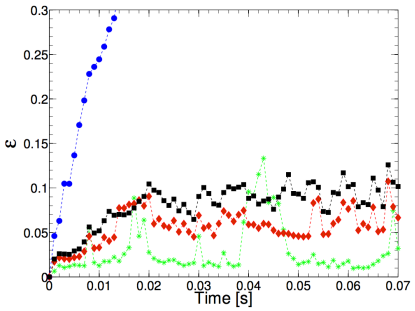

Fig. 1. Evolution of the overall error in a propane/air PaSR calculation between detailed representation, a 43-species (green) and a 34-species (blue) *single* reduced representations, and adaptive representations with an average of 30 (black) and 34 (red) species.

IV. Integration with ISAT/RCCE

The integration within the framework of Hiremath *et al.* follows in a straightforward manner. The size of the reduced representations are further decreased by introducing RCCE to complement species elimination provided by DRGEP, while for the reaction fractional step in flame simulation, separate ISAT tables are used for each region, reducing significantly the time to build the tables and accelerating the retrieval of reaction mappings.

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