

TABULATION-BASED SAMPLE-PARTITIONING ADAPTIVE REDUCED CHEMISTRY AND CELL AGGLOMERATION

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Abstract

In this study, we combine the SPARC (Sample-Partitioning Adaptive Reduced Chemistry) and the Cell Agglomeration (CA) techniques, to accelerate the simulation of laminar and turbulent reactive flows with detailed kinetics.

More specifically, the reduced mechanisms adopted by SPARC are generated on the basis of representative thermochemical states corresponding to laminar, steady-state flamelets parametrized by the mixture fraction and a progress variable, similar to the TRAC (Tabulated Reactions for Adaptive Chemistry) method, recently proposed by Surapaneni and Mira (*Comb. & Flame* 251, 2023). To further speed-up the calculation, CA (consisting in grouping the computational cells having similar thermochemical states during the chemical step) is carried out before identifying the local reduced mechanism by SPARC.

To demonstrate the effectiveness of the approach, we considered two benchmark cases: i) a laminar, pulsating laminar coflow diffusion flame fueled by a mixture of C_2H_4 and N_2 burning in air; ii) a 2D, turbulent, non-premixed flame burning $n-C_7H_{16}$ in air subject to decaying isotropic turbulence. In both cases, a detailed kinetic mechanism accounting for the formation of PAHs and soot particles and aggregates was considered. Preliminary numerical tests were conducted to investigate the feasibility of the proposed tabulation-based SPARC-CA methodology. The results are promising, showing both accuracy and computational efficiency, demonstrating the potential of the proposed methodology for advancing multi-dimensional CFD simulations of reactive flows with complex chemistry.

Introduction

In the pursuit of more effective design of combustion devices, such as industrial/domestic burners and gas turbines, detailed kinetics has emerged as a crucial factor for predictive simulations of laminar and turbulent flames. However, the computational coupling of Computational Fluid Dynamics (CFD) and detailed chemistry poses significant challenges, primarily due to the number of species

involved and the wide range of chemical timescales associated with complex chemistry [1]. While various acceleration techniques have been proposed during the years, the computational cost of CFD including detailed chemistry remains a concern, particularly for complex fuels.

CFD solvers based on the operator-splitting strategy are especially suitable for simulation of reactive flows with detailed kinetic mechanisms. In operator-splitting methods most of the computational time is spent to solve the chemical step, which consists in solving a number of independent, stiff, nonlinear systems of ordinary differential equations (ODEs), one per computational cell [2]. The independent nature of these ODE systems makes the application of adaptive chemistry techniques straightforward and highly effective. The core idea behind adaptive chemistry revolves around the observation that within small temperature and composition ranges, numerous species have negligible concentrations, and only a limited number of species remain chemically active. Consequently, the kinetic mechanism required to describe the chemical evolution within a specific thermo-chemical space may demand fewer species and reactions than the complete mechanism applicable to the entire thermo-chemical space. At the highest level of adaptivity and reduction, the local thermo-chemical state is evaluated *on-the-fly*, and a reduced kinetic mechanism is specifically generated in each computational cell (Dynamic Adaptive Chemistry) [3]. However, the computational cost associated to the reduction operations is substantial, especially for higher levels of reduction and complex mechanisms.

To alleviate the additional cost of adaptive reduction, the Sample-Partitioning Adaptive Chemistry (SPARC) approach was recently proposed and applied [4]. In SPARC, the *on-the-fly* mechanism reduction overhead is avoided, by building in a preprocessing phase a library of reduced mechanisms to be used in different regions of the domain during the CFD simulation. In SPARC, the challenge lies in effectively partitioning the composition space into clusters, ensuring that each cluster exhibits sufficient homogeneity from a kinetic point of view. Several approaches have been considered, from combination of Self Organizing Maps (SOM) with k-means to Principal Component Analysis (PCA).

In the present work we explore the possibility to use low-dimensional manifolds to identify regions with different chemical activities, in line with the TRAC (Tabulated reactions for adaptive chemistry) method, recently proposed in [5]. More specifically, we applied the pre-partitioning operations on representative thermochemical states corresponding to laminar, steady-state flamelets parametrized by the mixture fraction ξ and a normalized progress variable Y_c^n . The advantage over SOM or PCA is that the multi-dimensional data generated in the preprocessing phase are now linked to two control variables (ξ and Y_c^n) having a clear physical interpretation and direct connection with chemical kinetics.

To further speed-up the calculation, Cell Agglomeration (CA) was combined with SPARC. In CA, at each reaction step, the computational cells with similar properties, also called *features*, are grouped together in a single zone with averaged values. Chemistry calculations are carried out per zone (instead of computational cells) and

the results are mapped back to the original, individual cells. Since the number of zones is usually much smaller than the total number of cells, CA is expected to result in significant computational saving. Instead of using the temperature and selected key-species, the idea in this work is adopt ξ and Y_c^n as *features* in the agglomeration process, consistently with the SPARC algorithm.

In the next Section, the SPARC and CA techniques based on tabulated chemistry will be described with more details. Then, two examples of application of the proposed methodology will be presented and briefly discussed.

Methodology

The general idea behind the adaptive chemistry approach here proposed is the assumption that not all the species contained in a detailed kinetic mechanism are (locally) equally necessary. Depending on the physics of the reacting flow, a reduced set of species and reactions can be identified in each cell at each time step.

The proposed procedure consists of 2 phases. The first phase is carried out as a preprocessing step and consists of the following operations:

1. Dataset generation: the training dataset is constructed from the solutions of steady and unsteady adiabatic diffusion flamelets. The steady flamelets are simulated by varying the applied strain rate until an extinction limit. The composition space between the most strained flamelet and mixing limit is covered by using an unsteady formulation of flamelets.
2. Dataset parameterization: the generated database is remapped over two control variables, the mixture fraction ξ and the normalized progress variable Y_c^n , using a 401×401 grid with uniform spacing.
3. Partitioning of the thermochemical space: a clustering algorithm is adopted to identify in the $\xi - Y_c^n$ space continuous regions (i.e., clusters) having similar kinetic behavior. In the present work, for simplicity, the $\xi - Y_c^n$ space is decomposed in 40×40 clusters by means of a regular 2D grid. Thus, each cluster is uniquely identified by the ξ and Y_c^n values at its center.
4. Generation of reduced mechanisms: for each cluster of the dataset, a reduced mechanism is generated via the Directed Relation Graph (DRG) method [6]. The total number of reduced mechanisms is 1,600.

The second phase corresponds to the chemical step of the CFD simulation and consists of the three following operations:

1. Cell agglomeration: cells having similar thermochemical state (identified by ξ and Y_c^n variables only) are grouped together and their average mixture fraction $\bar{\xi}$ and progress variable \bar{Y}_c^n are estimated. The Dynamic Multi-Zone (DMZ) algorithm [7], which is based on an unsupervised evolutionary clustering algorithm which automatically determines the optimal number of clusters for a user-defined level of accuracy, is here adopted.
2. Identification of reduced kinetic mechanism and chemical integration: based on averaged $\bar{\xi}$ and \bar{Y}_c^n , the reduced kinetic mechanism in each cluster is identified from the library built in the preprocessing step. The conservation equations of

species and energy are then solved according to the reduced kinetic mechanism.

3. Back-mapping: the calculated thermo-physical state at the cluster level is mapped back to the original cells, using the backward remapping procedure proposed by Liang et al. [3], which ensures the conservation of mass.

Results and discussion

The first configuration chosen to test the proposed methodology is an axisymmetric, time-varying, non-premixed laminar coflow flame. The fuel is a mixture of 60% C_2H_4 and 40% N_2 (molar basis), while the oxidizer stream is regular air. Both streams are fed at ambient temperature and atmospheric pressure. A transient behavior was induced by a sinusoidal perturbation in the velocity profile of the fuel stream with frequency $f=10\text{ Hz}$ and amplitude $A=0.90$. Additional details can be found in [8].

The second configuration here adopted is the two-dimensional, turbulent, non-premixed flame burning a mixture of $n-C_7H_{16}$ and N_2 (0.844/0.156 by volume) in air subject to decaying isotropic turbulence, proposed by Bisetti et al. [9].

In both cases, the simulations have been carried out using a detailed kinetic mechanism developed by the CRECK Modeling Lab including the chemistry of PAHs (Polycyclic Aromatic Hydrocarbons) and accounting for the formation of soot particles and aggregates via a Discrete Sectional Method (DSM) [10], with a total number of species and reactions equal to 185 and $\sim 8,000$, respectively.

As mentioned in the previous section, the training dataset was built from the solutions of steady and unsteady adiabatic laminar flamelets, from a strain rate of $a=0.01\text{ 1/s}$ (close to thermodynamic equilibrium), to the extinction, corresponding to $a_q=250\text{ 1/s}$ (laminar coflow flame fed with C_2H_4) and $a_q=90\text{ 1/s}$ (turbulent diffusion flame fed with $n-C_7H_{16}$). The dataset was parameterized through the mixture fraction ξ and a progress variable Y_C^n defined as suggested in [5]. Figure 1 presents the maps of temperature and mass fractions of soot particles and aggregates stored in the training dataset as a function of ξ and Y_C .

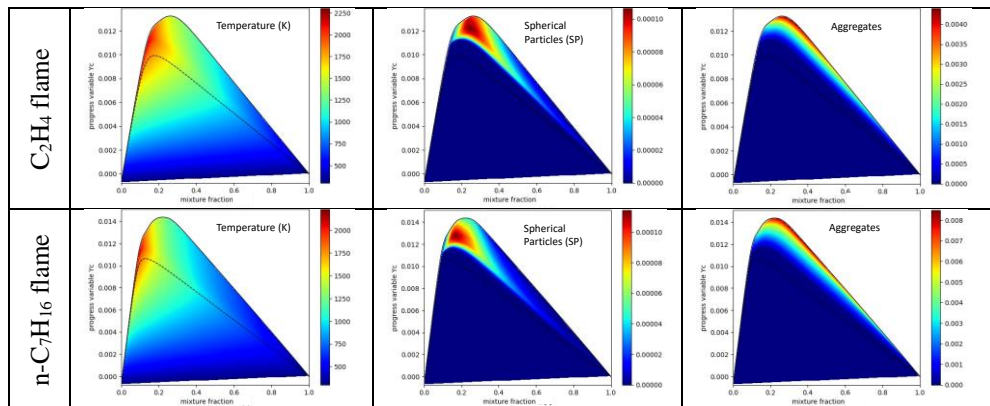


Figure 1. Temperature and soot mass fraction fields (spherical particles and aggregates) as a function of mixture fraction ξ and progress variable Y_C .

The chemical reduction was carried out as a preprocessing step using the DRG technique. In particular, for both the datasets, six key-species (fuel, O_2 , N_2 , OH , BIN5AJ and BIN13AJ) were selected and a tolerance $\varepsilon_{DRG} = 0.05$ was adopted. BIN5AJ and BIN13AJ are the discrete sections corresponding to the smallest soot spherical particle and the smallest soot aggregate. They were included in the set of key-species since to properly capture the soot kinetics during the reduction phase. Figure 2 presents the number of active species and reactions in the ξ - Y_C^n space and the regions where BIN5AJ is retained in the reduction process. A region of reduced mechanisms with high number of species and reactions is evident in the rich side, where the formation of soot is expected to be relevant (see Figure 1).

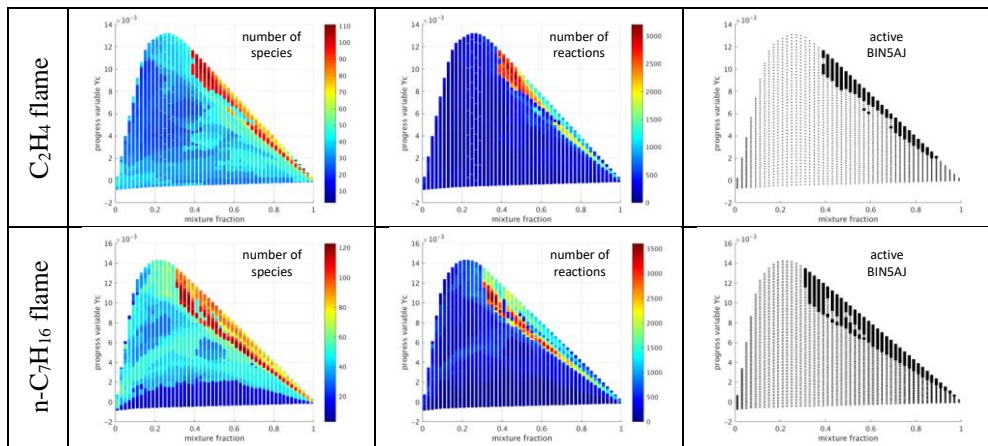


Figure 2. a, b) Maps of active species and reactions after the reduction process via DRG; c) regions (in black) where the pseudo-species BIN5AJ is retained.

The CFD simulations were carried out using the laminarSMOKE++ code [2]. The solutions calculated with the complete detailed kinetic mechanism are compared with those obtained from the application of the proposed methodology, which combines tabulated-based SPARC and CA (in which ξ and Y_C^n are assumed as features, with a tolerance $\varepsilon_{CA} = 0.01$). Figures 3 and 4 show the calculated fields of temperature and selected mass fractions at different times for the two benchmark cases. The agreement is quite good in both cases: the dynamics is well captured, and no significant deviations of the SPARC-CA results are evident, for temperature and soot.

In both cases here investigated, $\sim 95\%$ of total CPU time is spent for performing the chemical step when the complete kinetic mechanism is adopted. Thus, since the SPARC-CA method is able to accelerate the chemical step only, the maximum theoretical speed-up which can be achieved is ~ 20 . For the unsteady laminar coflow flame fed with C_2H_4 the measured average (over a single cycle of oscillation) speedup was ~ 16 (i.e., about 80% of theoretical maximum). Similarly, for the turbulent $n-C_7H_{16}$ flame, the average (in the 0-30 ms interval) speedup was ~ 15 (i.e.,

$\sim 75\%$ of theoretical maximum). As demonstrated in [7], the additional computational cost of CA is negligible with respect to the time for carrying out the chemical step (of the order of $\sim 1\%$). Since the partitioning is available as a 2D regular grid in the $\xi - Y_c^n$ space, the additional cost to identify the reduced kinetic mechanism is negligible, requiring only the local values of ξ and Y_c^n .

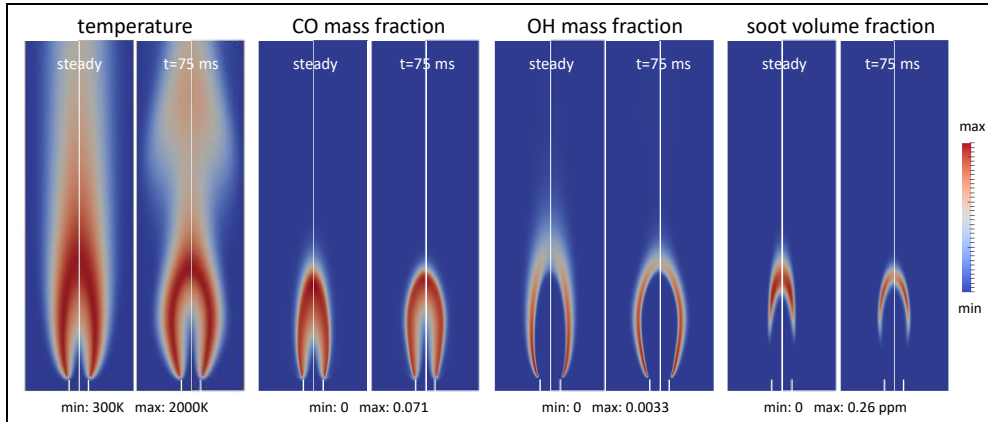


Figure 3. Calculated maps of T , mass fractions of CO and OH and soot volume fraction. Left sides: fully resolved solution; right sides: SPARC-CA solution.

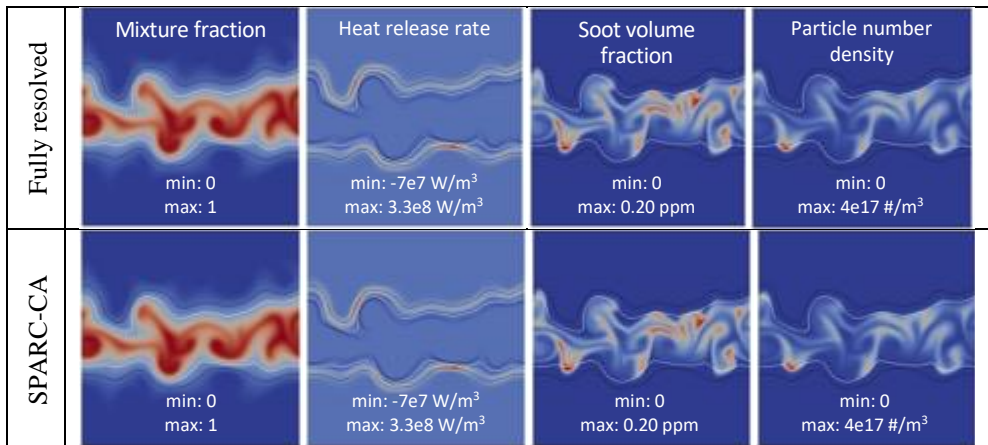


Figure 4. Maps of selected variables in the turbulent non-premixed flame fed with $n\text{-C}_7\text{H}_{16}$ at $t=10$ ms. The black and white lines identify the isolines $\xi = 0.143$ and $\xi = 0.3$, respectively.

Conclusions

In this work, we combined the SPARC (Sample-Partitioning Adaptive Reduced Chemistry) and the Cell Agglomeration (CA) techniques with tabulation of

chemistry in a 2D space, to accelerate the simulation of laminar and turbulent reactive flows with detailed kinetics. The proposed approach was applied to laminar and turbulent flames. The results, even if preliminary, are satisfactory: the accuracy is good in both the benchmark cases with good levels of acceleration, close to ~80% of theoretical maximum speed up. More systematic and complete analyses are required to better assess the performances and the limitations of the methodology. To conclude, the tabulation-based SPARC-CA method is a promising technique to accelerate simulations of reactive flows, especially considering that its implementation in operator-splitting-based CFD codes is very straightforward.

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