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Application of dynamic adaptive chemistry and in situ adaptive tabulation for computationally efficient modeling of supersonic turbulent combustion

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Abstract

To deal with the major challenges of combustion simulation with detailed chemical kinetics, dynamic adaptive chemistry (DAC) method and In Situ Adaptive Tabulation (ISAT) method were introduced to accelerate numerical calculation in supersonic turbulent combustion flows. The proposed methods were validated in a hydrogen fueled model scramjet combustor (DLR) with 9 species and 27 reactions, and a total of eight cases with different threshold values using large eddy simulation were set. Compared to the case without any acceleration method, the results indicate that the two proposed methods can accurately capture the flame structure, and that the relative percentage errors of temperature and species concentration are well-controlled and proportional to the threshold values. As for performance, detailed diagnostics show that DAC and ISAT with different threshold values reduce the computational overhead of ODE integration by factors of 1.4 to 1.71 and 2.1 to 4.0, respectively. The successful validation demonstrates that the two proposed methods can be efficiently used in the simulation of supersonic reactive flow for detailed kinetic mechanisms.

Keywords: *Dynamic adaptive chemistry, Mechanism reduction, ISAT; Turbulent combustion.*

1. Introduction

Renewed interests in hypersonic flight vehicles both for terrestrial travel and space exploration and transport have greatly motivated research effort towards supersonic combustors.

The development of these advanced combustion energy conversion systems requires accurate simulation tools, such as Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES), for ignition, combustion instability, lean blow-out, and emissions. However, accurate simulation with detailed chemical mechanisms describing the combustion process typically involves hundreds of species and thousands of reactions, and is thus extremely challenging, even with the most powerful computation facilities. Hence, numerous methods for chemistry integration have been developed to overcome this challenge. The developed methods mainly include one or more of the following four kinds of strategies. 1) Reduce the stiffness of ODE (ordinary differential equations) and improve ODE solvers [1,2]. 2) Agglomerate similar cells [3-5]. 3) Storage/retrieval methodologies [6-8]. 4) Reduce the size of chemical mechanisms [9-13]. The third and fourth strategies are the focus in this study.

In storage/retrieval methodologies, the ISAT (In Situ Adaptive Tabulation) method is a pivotal and typical approach for accelerating calculation. When ISAT is employed in a simulation, which can be used in DNS, LES, or RANS, the thermochemical states are tabulated in binary trees. Then, ISAT can subsequently reuse it and substantially reduce the cost of chemical integrations and speed up the

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calculations. The speedup obtained can increase when the simulation recalculates the same thermochemical states, e.g., the speedup factors achievable by a steady reactive flow are in the range 100–1000 [6]. However, for simulation of transient processes such as ignition and auto-ignition, the performance of ISAT decreases because the changing states inhibit reuse of the tabulated information. Strategies such as the cleaning strategy have been proposed to improve the efficiency [8]. As for mechanism reduction, this strategy employs either of two approaches to reduce the size of chemical mechanisms. One approach is to generate pre-reduced skeleton mechanisms using a method such as the multi-generation path flux analysis (PFA) method [14], the direct relation graph (DRG) method [15], or the DRG with error propagation (DRGEP) method [16]. However, the pre-reduced mechanisms typically have to be produced based on a fixed condition or several interested conditions. To avoid this problem, another approach, in which locally reduced mechanisms are generated for each grid and time step based on local thermodynamic condition, can be applied by utilizing either an adaptive chemistry (AC) method [9] or a dynamic adaptive chemistry (DAC) method [12, 13].

The DAC approach was first proposed by Liang et al. [13] for homogeneous ignition scenarios, where the basis of mechanism reduction is achieved through the DRGEP method. Using DAC, a small skeletal mechanism that is valid for the local thermochemical condition is obtained for each cell and time step. This procedure removes unimportant species from the detailed mechanism and freezes their mass fractions in the subsequent computation, resulting in reduction of the ODE system and acceleration of the computation. Contino et al. [10] subsequently combined ISAT and DAC and simulated the highly efficient IC engine with detailed chemistry. The ISAT-DAC (TDAC) method can speed up calculations by factors in the range of hundreds to thousands with accurate results for species mass fraction, temperature, and emissions. However, These methods have not been validated in supersonic turbulent combustion flows.

In this study, dynamic adaptive chemistry (DAC) method and In Situ Adaptive Tabulation (ISAT) method were introduced to accelerate numerical calculation in supersonic turbulent combustion flows. The remainder of this paper is organized as follows. Section 2 introduces the two methods. Section 3 briefly describes test cases and the numerical approach. Section 4 presents performance analyses conducted of DAC and ISAT. Section 5 concludes this paper.

2. Method

To simulate a reactive flow, a CFD solver needs calculate the integration of chemical reactions of overall computational cells to obtain the thermochemical compositions alteration. In general, the thermochemical state of the mixture (at a given position and time) is completely characterized by the pressure p, the mixture sensible enthalpy h_s, and the vector $\boldsymbol{Y}$ of species mass fractions, i.e $\boldsymbol{\phi} \equiv \{\boldsymbol{Y}, h_s, p\}$

With a Strang-based splitting scheme, integration of chemical reactions is separated from that of other physical processes, e.g. diffusion and advection. Then the φ of each computational cell during chemistry reaction fractional steps evolves according to a set of nonlinear ODEs in which chemical source term is governed by

$$d\boldsymbol{\phi}/dt = \boldsymbol{S}(\boldsymbol{\phi}) \tag{1}$$

where $\boldsymbol{\phi}$ is the vector of local thermochemical compositions and $\boldsymbol{S}$ is its rate of change due to chemical reactions. To determine the thermochemical composition altered by chemical reactions over a time step, the CFD solver loops over all the computational cells and calculates the integration of each reaction step, typically using stiff ODE solvers. However, the numerical integration of the large number of such ODEs is computationally expensive.

Therefore, to speed up the integration, the basic idea of the DAC is to generate locally reduced kinetics for each spatial and time step.

Using DAC, a small skeletal mechanism that is valid for the local thermochemical condition is obtained for each cell and time step. This procedure removes unimportant species from the detailed mechanism and freezes their mass fractions in the subsequent computation, resulting in reduction of the ODE system and acceleration of the computation. The current mechanism reduction is conducted by directed relation graph with error propagation (DRGEP) algorithm [13], which determines the

linking strength of a target specie to the user defined search initiating set of species while considering the error damping process in the reaction network. The DRGEP method finally extracts a set of active species and their associated elementary reactions based on the local thermochemical states and them error threshold ε DAC. To maintain the consistency during the mechanism switch, the ODE associated with those disabled species are not solved, whereas their concentrations are still considered when involved in the three-body and pressure-dependent reactions. The previous applications of DRGEP-based DAC [12,13] have proved the high efficiency yet adequate accuracy through the synergy of tabulation and dynamic mechanism reduction scheme

The ISAT (In Situ Adaptive Tabulation) method is a pivotal and typical approach for accelerating calculation. When ISAT is employed in a simulation, during the integration of the species-evolving ODE system over the current time-step, a query composition vector ψ_q is firstly provided to the tabulation layer. The ISAT module will try to retrieve a previously stored result of reaction mapping $R(\psi_0)$ within the local error threshold ε(ISAT) and linearly estimates the current reaction mapping as $R(\psi_0)$. If the query is not retrievable within the current ellipsoid of accuracy (EOA), direct integration of the stiff ODE system will be applied and the binary tabulation tree will be expanded by adding a new leaf or growing the current leaf depending on whether the local error exceeds the ε(ISAT). The pressure as a status variable is also stored in the ISAT table since the constant pressure assumption is no longer valid for transient supersonic flows with high compressibility. Although similar to the treatment in the internal combustion engine simulation [13], the setup is much more challenging. In the previous engine simulations, pressure changed widely over the entire simulation but without dramatic change within the computational domain, mostly because it was homogeneous charge compression ignition. In supersonic flows, discontinuity induced by shock waves in the domain is much stronger and more complex to handle for ISAT.

Besides, all the work presented in this paper is based on a well-established numerical flow solver, OpenFoam —a C++ library capable of DNS/LES/RANS of reacting and non-reacting flows using the unstructured collocated finite volume method (FVM) [17], in which the discretization was based on Gauss theorem. This code has been applied to a range of flow problems, including non-reacting flows, and reacting flows, usually with good agreement with experimental data.

3. Test cases

To demonstrate the accuracy and efficiency of the proposed methods, a hydrogen fueled model scramjet combustor (DLR) were simulated. The DLR [17] configuration had a one-sided divergent channel (length: 340 mm, inlet cross-section: 45 × 50 mm, wedge tip at X = 35 mm, Y = 25 mm). The air enters the inlet at Mach 2 and hydrogen is injected from the base of the wedge (with angle 12 degrees) through four holes. A 2D LES parallel simulation with 9 species 27 reactions [18], 24 processors and one million cells (44780 cells per processor) was conducted. The CFL number was less than 0.3, corresponding to a physical time step of 1×10-7 s.

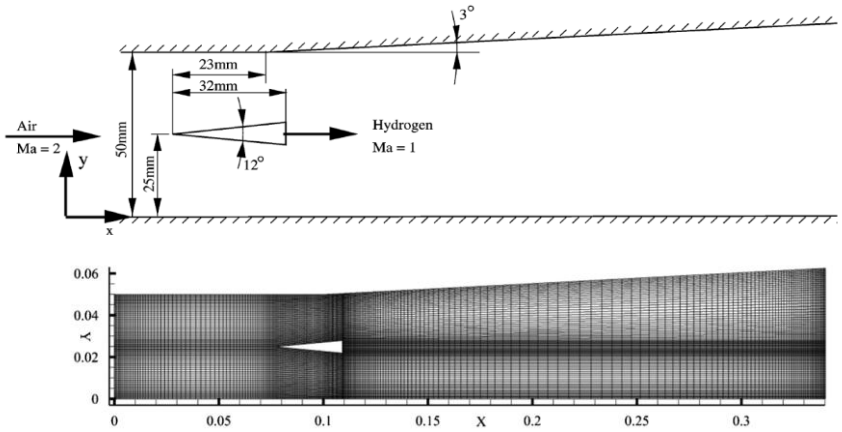

Fig 1. A schematic view of DLR configuration and meshes

Table 1. Inflow conditions for the air stream and hydrogen jet of DLR configuration

	Ma	Temperature/K	Pressure /Pa	O2	N2	H2O	H2
Air	2.0	340	100	0.232	0.736	0.032	0
H2	1.0	250	100	0	0	0	1

This configuration with strong chemistry-transport coupling was designed to illustrate the accuracy and performance of the proposed method. To achieve this goal, eight cases with different threshold values were set and can be found in Table 1. The ODE case represents a case without any acceleration method, and was used as a benchmark for the simulation of each configuration.

Table 1. Test cases for DLR

Methods	**Cases name**	**Threshold values**
ODE	0	-
DAC	1	1E-1
	2	1E-2
	3	1E-3
	4	1E-4
ISAT	5	1E-4
	6	5E-5
	7	1E-5
	8	5E-6

4. Results and discussion

4.1. Accuracy analysis

As shown in Fig. 1, the recirculation region serves as a flame holder for the H2 diffusion flame with combustion. The oblique shock wave formed by the leading edge of the strut continuously reflects with the wall of the combustion chamber and the shear layer of the wake of the strut, forming a series of oblique shock waves along the flow direction. As the flow progresses, the shear layer of hydrogen and incoming air becomes thicker, and the heat release zone and the high temperature zone are increased. Compared to the case without any acceleration method (case 0), there is no observable difference between the different cases for temperature contours. A similar situation is seen in Fig. 2, the contours of pressure of different cases are anastomotic. These results indicate that the two proposed methods can accurately capture the flame structure.

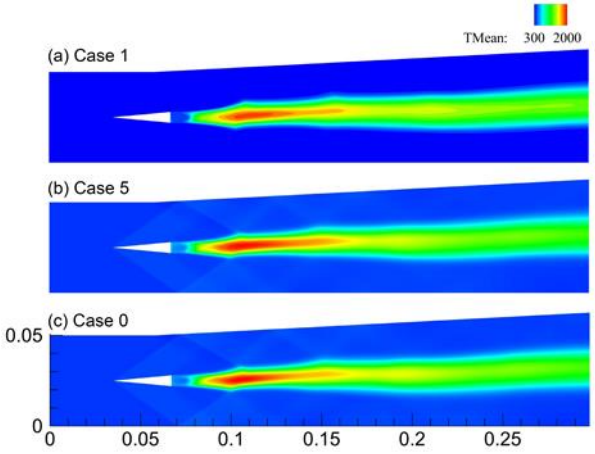

Fig 2. Contours of temperature of case 1, case 5 and case 0.

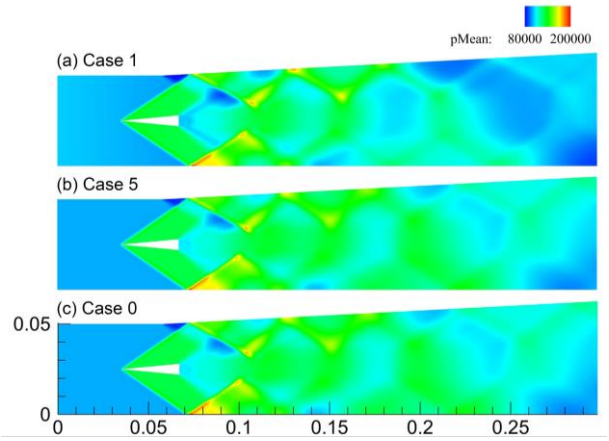

Fig 3. Contours of pressure of case 1, case 5 and case 0.

Because there is no observable difference between the cases, the consistency was further assessed via more quantitative comparisons. We measured the average relative percentage errors incurred in the selected phase parameters. To further verify that the methods can provide accurate and reliable results, we measured the relative percentage errors incurred in the selected phase parameters, which are defined as follows:

$$\eta = \frac{|\varphi - \varphi^{ODE}|}{\varphi^{ODE}} \times 100\% \tag{2}$$

where φ is a quantity of interest, e.g. temperature.

Fig. 3 shows the relative percentage errors of temperature and pressure with different cases. The results show that the relative percentage errors of the DAC cases with different thresholds is not much different, around 1.25% for mean temperature and 0.9 % for mean pressure. This is mainly because the mechanism of hydrogen is small. As for ISAT cases, the relative percentage errors of case 6 is the smallest, and this threshold value seems to be an optimal solution. However, the threshold value sensitivity of the ISAT method is greater than the DAC method; an excessive threshold value of the ISAT can even distort the result. This is mainly due to the strong discontinuity in the supersonic field - shock waves.

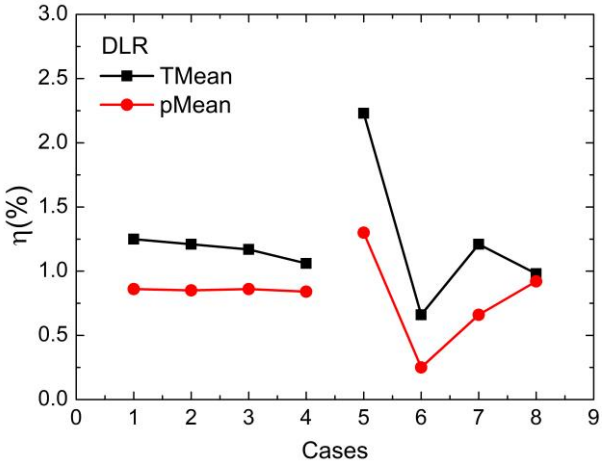

Fig 4. Relative error in temperature and pressure of different cases.

4.2. Performance analysis

In addition to accuracy, performance is also emphasized in the new methods. The average number 嗯 active species of different DAC cases are given in the first row of Table 2. The results show that the difference in the active species of different threshold is small. As mentioned before, because of the small mechanism of hydrogen, it is difficult to further simplified. therefore, as shown in Fig. 6, the speedup factors of DAC cases are around 1.5.

Table 2. Calculation parameters

Cases	ODE	1E-1	1E-2	1E-3	1E-4
DAC active species	10	7.81	7.97	7.98	8.31
Cases	ODE	1E-4	5E-5	1E-5	5E-6
ISAT retrieval (%)	-	96.9	87.8	79.2	65.1

Figure 5 shows the distribution of the ISAT operations for the four ISAT cases. The red area represents the retrieval operation, which means that the data is found from the stored table. The green area and the blue area represent the growth EOA and the addition respectively, and need a direct integral. The fourth line of Table 2 gives the percentage of ISAT retrieval. From the results, the retrieval was carried out for most areas in case 5. In the case 6, case 7 and case 8, 87.8%, 79.2% and 65.1% of the grids are retrieved, respectively. On the whole, most of the flow fields that have not undergone chemical reactions are retrieved. The main difference lies in the burning area where the chemical reaction is severe. The main difference between the different cases is the part of the wake of the strut in the rear part of the combustion chamber.

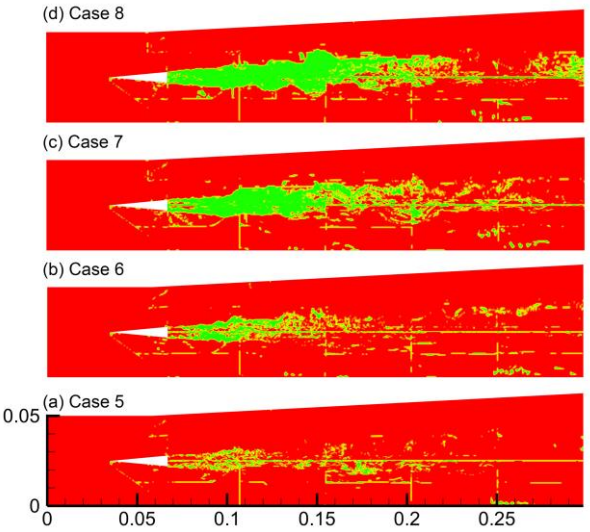

Fig 5. The distribution ISAT retrieval

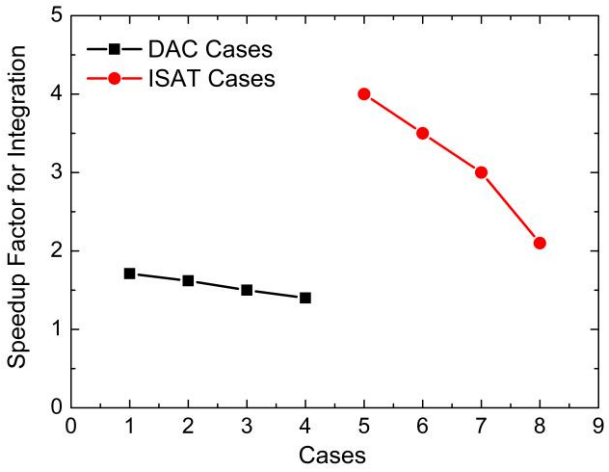

Fig 6. Average (entire field) speedup factors for integration

As for performance, detailed diagnostics show that DAC and ISAT with different threshold values reduce the computational overhead of ODE integration by factors of 1.4 to 1.71 and 2.1 to 4.0, respectively. The speedup factor obtained by the DAC is less affected by the threshold, and is also smaller than that of the ISAT, mainly due to the small mechanism of hydrogen. For the ISAT method, 5e-5 is a suitable threshold that can balance accuracy and speed. The successful validation demonstrates that the two proposed methods can be efficiently used in the simulation of supersonic reactive flow for detailed kinetic mechanisms.

5. Conclusions

In this paper, two chemical reaction acceleration methods are used: DAC and ISAT. The large eddy simulation of the DLR configuration supersonic combustor is carried out, and compared with the ODE method and experimental data. The main conclusions are as follows: 1. The calculation results of ODE, DAC and ISAT method are in good agreement with the experimental results, and the numerical method is reliable. 2. The two methods can be used for numerical simulation acceleration in supersonic combustion, which can effectively improve the numerical simulation efficiency and speed up the calculation of chemical reaction. Compared with the ODE direct integration method, the overall acceleration is about 3.5 times.

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