



The use of dynamic adaptive chemistry and tabulation in reactive flow simulations



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ABSTRACT

Detailed chemical kinetics is an integral component for predictive simulation of turbulent flames and is important for reliable prediction of flames and emissions. Major challenges of incorporation of detailed chemistry in flame simulations are induced by the large number of chemical species and the wide range of timescales involved in detailed kinetics. In this work, dynamic adaptive chemistry (DAC) and in situ adaptive tabulation (ISAT) for efficient chemistry calculations in calculating turbulent reactive flows with detailed chemistry are studied in iso-octane/air homogeneous charge compression ignition (HCCI) and methane/air combustion in a partially-stirred reactor (PaSR). Chemistry calculations are accelerated by DAC via expediting the integration of ordinary differential equations (ODEs) governing chemical kinetics with local skeletal mechanisms obtained on-the-fly using the directed relation graph (DRG) method, and by ISAT via reducing the number of ODE integrations through tabulating and re-using the ODE solutions. It is shown that, in contrast to ISAT, the performance of DAC is mostly independent of the nature of combustion simulations, e.g., steady or unsteady, premixed or non-premixed combustion, and its efficiency increases with the size of chemical kinetic mechanisms. DAC is particularly suitable for transient combustion simulations with large mechanisms containing hundreds of species or more, such as those for gasoline or diesel fuels. A speedup factor of about 30 is achieved for HCCI combustion of iso-octane/air with good agreements in the histories of temperature and species concentrations. In contrast, ISAT performs better for simulations where chemistry calculations can be predominantly resolved by retrieving from the ISAT table, i.e., re-using the ODE solutions. It is shown that ISAT achieves speedup factors of about 100 with only about 10%, 0.1% and 0.01% incurred errors in NO, CO, and temperature, respectively, for the premixed methane/air PaSR simulations. Moreover, a coupled DAC and ISAT approach, namely ISAT–DAC, has been developed and demonstrated in this study to accelerate chemistry evaluation. It is shown that the incurred errors in temperature and species concentrations in ISAT–DAC are well controlled, and it can significantly enhance the performance of ISAT, when the fraction of direct ODE integration is significant, via accelerating the ODE integrations by DAC.

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1. Introduction

Detailed chemical kinetics is an integral component for predictive simulations of turbulent flames and is important for reliable prediction of flames and emissions. Major challenges to incorporate detailed chemistry in flame simulations are induced by the large number of chemical species and the wide range of timescales involved in detailed kinetics [1]. In this study, we consider a react-

ing gas-phase mixture consisting of n_s chemical species, composed of n_e elements. The thermo-chemical state of the mixture at a given location and time is determined by the pressure p , the mixture sensible enthalpy h_s , and the n_s -sized vector \mathbf{Y} of species mass fractions. In a reacting flow computation, the species composition evolves through three processes: advection, diffusion and chemical reaction. Here we focus on the general class of solution methods in which a splitting scheme is used to account for these processes in separate fractional steps. The split equations are time-integrated separately and assembled in the end to approximate the full equations at each time step [2–10]. With chemical reactions being separated into a single (adiabatic and isobaric) reaction fractional step, the composition $\Phi \equiv \{\mathbf{Y}, h_s\}$ of each computational cell/particle during this sub-step evolves according to a set of nonlinear stiff or-

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dinary differential equations (ODEs) resulting from chemical kinetics,

$$\frac{d\Phi}{dt} = \mathbf{S}(\Phi), \quad (1)$$

where \mathbf{S} is the rate of change due to chemical reactions. The task in this reaction fractional step is to determine the thermo-chemical composition due to chemical reactions over a time step Δt . The time step, typically determined by the flow field, may be constant in space and time, or a variable with a typical range spanning several orders of magnitude.

With detailed chemical kinetics, the major computational challenge is the time-intensive nature of solving Eq. (1). A realistic description of combustion chemistry for hydrocarbon fuels typically involves tens to thousands of chemical species, and the time-scales can range from sub-nanoseconds to seconds [1]. In the past decade, significant progress has been made in methodologies and algorithms to reduce the computational cost imposed by the use of detailed chemistry in reactive flow simulations, and the frequently used approaches include: the development of skeletal mechanisms from large detailed mechanisms by the elimination of inconsequential species and reactions [11–18]; dimension-reduction techniques [19–29]; and storage/retrieval methodologies [30–35] such as in situ adaptive tabulation (ISAT) [33,34]; cell agglomeration methods such as multi-zone models [36–38]; and dynamic adaptive chemistry (DAC) [39–42]. In this study, we first investigate the relative performance of DAC and ISAT in the probability density function (PDF) [43] of turbulent flames, in which the chemical composition in the computational domain is represented by a large number of particles. Then we focus on exploring the combined DAC and ISAT methodology for PDF simulations, which enables us to extract the best out of the two methods, thereby further reducing the cost of chemistry computations.

When ISAT [33,34] is employed to speed up chemistry calculations in simulations, which can be direct numerical simulations (DNS), large eddy simulations (LES) or a PDF method, the task performed by ISAT in the reaction fractional step is to determine the cell/particle thermochemical compositions after a computational time step (either variable or constant) due to chemical reactions. By tabulating useful information in binary trees, i.e. the ISAT tables, and reusing it, ISAT can substantially reduce the number of direct chemical kinetic integrations and significantly speed up the chemistry calculations. The computational efficiency of the ISAT algorithm is higher when the tabulated information can be re-used more frequently. For instance, speedup factors of 100–1000 can be achieved using ISAT for statistically stationary reactive flows [33]. The performance of ISAT deteriorates when the accessed composition space keeps on changing such that the pre-tabulated entries can rarely be re-used, e.g., when simulating the transient auto-ignition processes in compression ignition engines. Specific improvements such as a cleaning strategy for infrequently accessed tabulated points [44] have been proposed to improve the ISAT efficiency. In this study, we explore the possibility to accelerate chemistry calculation using ISAT combined with dynamic adaptive chemistry (DAC).

The DAC approach [39–42] was first proposed by Liang et al. [39] to accelerate the time-integration of Eq. (1) through the use of locally (spatially and temporally) valid skeletal mechanisms. In [39–41] DAC was achieved through the directed relation graph with error propagation (DRGEP) method [14], which was invoked for each CFD cell to obtain a small skeletal mechanism that is valid for the local thermochemical condition. By using the DAC, only a small subset of species and reactions in the full mechanism were retained to capture the dominant reaction pathways for each local condition. Consequently, the ODE system governing chemical kinetics during the reaction fractional step is reduced in size due

to the eliminated unimportant species. DAC has been successfully demonstrated in internal combustion engine (ICE) simulations [39–41]. More recently, DAC has been demonstrated in PDF calculations of turbulent reactive flow simulation [42], where on-the-fly mechanism reduction is achieved through the directed relation graph (DRG) method [11,12] instead of DRGEP. Compared to DRGEP, DRG effectively controls the worst-case reduction error for all the species such that the selection of the threshold value is very simple.

The combined use of ISAT and DAC was first proposed by Contino et al. [45] for highly efficient IC engine simulations with detailed chemistry. A speed-up factor of hundreds to thousands was reported in subsequent IC engine simulations [45–47] with accurate predictions of species concentration, heat release and emission profiles. The focus of the present study is to explore the combined DAC and ISAT methodology for PDF simulations of general turbulent flames. To achieve this, the relative performance of DAC and ISAT is first investigated in PDF simulations of methane/air combustion in a partially-stirred reactor (PaSR) with various levels of computational complexities. Then the methodology and test results, including the reduction in simulation time and the loss in accuracy, for the combined use of DAC and ISAT for efficient chemistry calculations are reported. The major contributions of this work include a detailed performance comparison of DAC and ISAT in flame calculations with different computational complexities and the development of a coupled ISAT–DAC method. Compared to the coupled method in [45–47], the major differences and improvements include a more generalized specification of the search-initiating species in DAC, the use of a state-of-the-art ISAT algorithm [34], and an improved method for computing the sensitivity matrix needed for the coupled ISAT–DAC approach.

As an outline of the paper, the ISAT algorithm and the DAC approach will be reviewed in Section 2. Their relative performances in HCCI and PaSR are studied in Section 3. The integration of DAC and ISAT is formulated and investigated in Section 4. Conclusions are presented in Section 5.

2. Computationally-efficient implementation of chemistry using ISAT and DAC

2.1. Overview of the ISAT algorithm

The purpose of ISAT is to tabulate a function $\mathbf{f}(\mathbf{x})$, where \mathbf{x} and \mathbf{f} are of dimensions n_x and n_f respectively. Given a query with \mathbf{x}^q as input, ISAT returns $\mathbf{f}^q(\mathbf{x}^q)$ as an approximation to $\mathbf{f}(\mathbf{x}^q)$ if possible. An essential aspect of ISAT is that the table is built-up in situ, or at runtime, as the simulation is being performed, not in a pre-processing stage. The table is empty at the beginning of the simulation. Table entries, also referred to as leaves, are added as needed based on the queries, \mathbf{x}^q , generated by the simulation. As such, only the compositions accessed during the simulation need to be tabulated. The tabulated information on the n th leaf includes its location, $\mathbf{x}^{(n)}$, the function value, $\mathbf{f}^n = \mathbf{f}(\mathbf{x}^{(n)})$, and the $n_f \times n_x$ Jacobian matrix, $\mathbf{A}^{(n)}$, defined as $A_{ij} = \partial f_i / \partial x_j$. The \mathbf{A} matrix is used to construct the linear approximation employed in ISAT. Given a query, \mathbf{x}^q , the linear approximation to $\mathbf{f}(\mathbf{x}^q)$ on the n th leaf is

$$\mathbf{f}^{l,n} = \mathbf{f}^n + \mathbf{A}^{(n)}(\mathbf{x}^q - \mathbf{x}^{(n)}), \quad (2)$$

and the error in this approximation is

$$\varepsilon^{(n)}(\mathbf{x}^q) = \|\mathbf{f}^{l,n}(\mathbf{x}^q) - \mathbf{f}(\mathbf{x}^q)\|. \quad (3)$$

It is assumed that \mathbf{f} and \mathbf{x} are normalized, such that the two-norm is an appropriate measurement of the approximation error. Given a small error tolerance, $\varepsilon_{\text{ISAT}}$, ISAT returns an approximation to $\mathbf{f}(\mathbf{x})$ with errors, ε , which are (with reasonable probability) less than

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