



Dynamic adaptive acceleration of chemical kinetics with consistent error control

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ABSTRACT

The incorporation of detailed chemistry in combustion simulations is challenging due to the large number of chemical species and the wide range of chemical timescales. The performance of acceleration methods such as tabulation/retrieval strategies may deteriorate dramatically when large variation in the accessed composition space is present. In this study, a dynamic adaptive acceleration method (DAAM) is proposed, in which *in situ* adaptive tabulation (ISAT) or dynamic adaptive chemistry (DAC) is dynamically selected for chemistry integration based on the encountered composition inhomogeneity. The principle component analysis (PCA) of instantaneous representative compositions is employed to identify a low-dimensional subspace, in which the composition inhomogeneity of the computational cells is quantified through reconstructing the histogram of composition. ISAT is invoked for cells being in composition regions with high cell/particle numbers to avoid unnecessary tabulations and DAC is employed for the remaining ones by invoking on-the-fly reduction to generate small skeletal mechanisms for local thermo-chemical conditions and therefore accelerates the chemistry integration. A heuristic approach that dynamically adjusts the DAC reduction threshold based on the user-defined ISAT error tolerance has been proposed for DAAM, which enables a single, intuitive error control parameter for the combined use of these two methods and more importantly enables rigorous local error control. DAAM have been demonstrated in internal combustion engine (ICE) model simulations and premixed charge compression ignition (PCCI) engine simulations of *n*-heptane/air mixture, respectively. DAAM can improve the acceleration performance up to 50% compared to standalone ISAT while maintaining the same level of accuracy in temperature and species. It also shows advantage in speedup performance over the fixed ISAT-DAC method at the same level of accuracy.

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1. Introduction

Over the past several decades, the exploding development of detailed kinetics for hydrocarbon fuels [1,2] facilitates the reliable prediction of near-limit flame phenomena such as local extinction, re-ignition and emission characteristics in turbulent combustion simulations [3–10]. However, the time-intensive nature of integrating detailed chemistry due to the large number of chemical species and the wide range of chemical timescales poses a great computational challenge for multi-dimensional simulations, which may be further aggravated by the highly transient nature of the combustion processes such as those in internal combustion engines (ICE) [10].

Significant progress has been made in the development of numerical schemes and chemistry acceleration methods to efficiently accommodate detailed chemistry in combustion simulations [11–13]. For example, operator splitting schemes [14–16] have been employed to separate the time advancement of the governing partial differential equations into reaction and transport fractional sub-steps, such that efficient implicit ordinary differential equation (ODE) solvers such as DDASAC [17] can be applied for the chemistry integration. Operator splitting has been widely employed in large eddy simulation and (unsteady) Reynolds Averaged Navier–Stokes simulations and it allows the use of typical time steps of 10^{-6} s to 10^{-4} s, which are in general several orders of magnitude larger than the smallest chemical timescales.

Without loss of generality, one considers an isobaric and adiabatic reaction fractional step. The thermo-chemical state is described by the n_s -sized species mass fraction \mathbf{Y} and mixture sensible enthalpy h_s , i.e., $\phi \equiv \{\mathbf{Y}, h_s\}$, which evolves according to the

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following set of ODEs

$$\frac{d\boldsymbol{\phi}(t)}{dt} = \mathbf{S}(\boldsymbol{\phi}(t)), \quad (1)$$

where \mathbf{S} is the reaction source term governed by chemical kinetics. The task for the reaction substep is to compute the reaction mapping $\mathbf{R}(\boldsymbol{\phi})$, where $\boldsymbol{\phi}$ is the thermo-chemical state of a computational cell/particle at the beginning of the reaction time step of duration Δt , and \mathbf{R} represents the composition at the end of the integration step. The direct evaluation of $\mathbf{R}(\boldsymbol{\phi})$ involves integrating the stiff ODEs in Eq. (1) for a time Δt , which is computationally expensive. Various approaches have been proposed to accelerate chemistry calculation, which include the development of fast ODE solvers [18–20], dimension reduction [21–30], dynamic adaptive chemistry (DAC) [31–36], and storage/retrieval methods [37–41], etc. For example, dimension reduction methods such as skeletal mechanism [21–23], quasi-steady-state assumption [24], computational singular perturbation [25], rate-controlled constrained-equilibrium [26], intrinsic low-dimensional manifolds [28], the methods of invariant manifold [29], etc., globally reduce the dimension of the chemical kinetics and therefore accelerate the chemistry integration. In contrast, DAC invokes on-the-fly reduction to generate small skeletal mechanisms for local thermo-chemical conditions and thereafter reduces the size of ODEs and the integration time. The performance of DAC is found to be independent of the nature of the combustion simulations, and its efficiency increases with the increasing mechanism size [42]. For storage/retrieval methods such as *in situ* adaptive tabulation (ISAT) [40,41], they expedite the integration of Eq. (1) by tabulating the reaction mappings $\mathbf{R}(\boldsymbol{\phi})$ and reusing them for similar initial composition. Given a query with $\boldsymbol{\phi}^q$ as input, ISAT returns a linear approximation to $\mathbf{R}(\boldsymbol{\phi}^q)$ if possible, with the error being controlled by user-specified error tolerance. The efficiency of ISAT gets higher when the tabulated information can be re-used more frequently, i.e. for simulations of statistically steady state flames. However its performance deteriorates dramatically in ICE simulations which are highly transient process with large pressure variations and the accessed composition space keeps on changing such that the pre-tabulated entries can rarely be re-used [43].

The combined use of different acceleration methods has become a trend to achieve higher efficiency of combustion simulations. DAC and dimension reduction methods have been routinely employed in combination with tabulation methods to accelerate the necessary chemistry integration by reducing the number of representative species solved during integrations [9,42,44–47]. Currently, in general, a fixed acceleration strategy (through either standalone or combined acceleration methods) is employed for all the encountered compositions throughout an entire simulation. For example, a combined approach named ISAT-DAC, or TDAC, was proposed for efficient ICE simulations [44] and later extended for general turbulent combustion simulations [42,45]. In ISAT-DAC, DAC is invoked to expedite the expensive chemistry integrations for adding new entries or failed retrieval attempts in ISAT through removing unnecessary species and reactions based on the locally encountered composition. ISAT-DAC has been demonstrated to achieve a speedup factor of hundreds to thousands for near-homogenous engine simulations [44] and statistically stationary turbulent flames with small or moderate sized chemical mechanisms [42]. However its performance may deteriorate dramatically under engine conditions with large pressure variation and composition inhomogeneity because the new entries added during the combustion stage cannot be reused as many times to pay off the computational overhead [43,45].

As reported in [10], a fixed acceleration strategy may not be optimal for combustion simulations with large variation in pressure and composition. A static adaptive chemistry acceleration

approach has been proposed and preliminarily explored [10], in which the acceleration method e.g., ISAT or DAC is employed at different combustion stages based on the encountered composition inhomogeneity and reaction activity. Specifically, ISAT is employed during the compression and post-combustion stages in which composition inhomogeneity is in general not significant, and DAC is employed during the combustion stage. For a simulated HCCI combustion with heat loss, the static adaptive approach is found to be three times more efficient than ISAT-DAC while maintaining the same level of accuracy in predictions, demonstrating the greater potential of adaptive acceleration approaches than the fixed strategies. However, the specification of acceleration methods for different stages in the static method is empirical and is hard to be extended to general combustion simulations. In addition, at a given time instance, either ISAT or DAC is employed for all the encountered cell/particle compositions in the computational domain, which may not be optimal for efficiency.

Another important issue of the combined approach, which is rarely addressed, is the consistent error control. The error control strategies of various acceleration methods may be dramatically different from each other. In a combined approach, at least two separate error control parameters, in general without any correlation, are needed to be specified, which adds significant extra efforts to determine the proper settings for a combustion simulation. For example, for DAC, the extent of local reduction is controlled by the user-specified reduction threshold ε_{DAC} . The accuracy in reaction mapping depends on reduction threshold, initial composition, the integration time step and possibly other parameters such as starting species. There is in general no intuitive relation between reduction threshold and the local error in reaction mapping. This is dramatically different from ISAT, in which the error tolerance ε_{ISAT} directly controls the accuracy in reaction mapping. Consequently when applying ISAT-DAC for turbulent combustion simulations, the proper settings of DAC reduction threshold and ISAT error tolerance have to be determined through a trial and error procedure in the two-dimensional parameter space that may involve many calculations of model problems such as partially-stirred reactor simulations at representative conditions [42], which adds significant computational cost.

In this study, a dynamic adaptive acceleration method (DAAM) is developed for the optimal use of ISAT and DAC for chemistry acceleration. In addition, a consistent error control strategy of ISAT and DAC is proposed so that a single error tolerance is employed that controls the local incurred error in composition. This is the first attempt that addresses both the dynamic adaptive acceleration and consistent error control for the combined acceleration approach. With DAAM, at a given reaction fractional step, for each individual computational cell/particle, it dynamically selects the optimal acceleration method based on the encountered composition inhomogeneity, which is quantified through reconstructing the histogram in a low-dimensional composition subspace determined by principle component analysis (PCA) [48]. The histogram is obtained by counting up the number of particles/cells fall into each grid in the subspace. ISAT is invoked for computational cells in regions with high cell/particle numbers to avoid unnecessary tabulations that would be rarely reused. DAC is employed to accelerate chemistry calculations for the remaining ones by invoking on-the-fly reduction to generate small skeletal mechanisms for local thermo-chemical conditions. The rest of paper is organized as follows. In Section 2, the methodology of DAAM is elaborated with emphasis on characterization of composition inhomogeneity and consistent error control. In Section 3, its performance is analyzed in ICE model simulations with various levels of composition inhomogeneity and PCCI engine simulations. Conclusions are in Section 4.

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