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Dynamic adaptive chemistry with operator splitting schemes for reactive flow simulations



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ABSTRACT

A numerical technique that uses dynamic adaptive chemistry (DAC) with operator splitting schemes to solve the equations governing reactive flows is developed and demonstrated. Strang-based splitting schemes are used to separate the governing equations into transport fractional substeps and chemical reaction fractional substeps. The DAC method expedites the numerical integration of reaction fractional substeps by using locally valid skeletal mechanisms that are obtained using the directed relation graph (DRG) reduction method to eliminate unimportant species and reactions from the full mechanism. Second-order temporal accuracy of the Strang-based splitting schemes with DAC is demonstrated on one-dimensional, unsteady, freely-propagating, premixed methane/air laminar flames with detailed chemical kinetics and realistic transport. The use of DAC dramatically reduces the CPU time required to perform the simulation, and there is minimal impact on solution accuracy. It is shown that with DAC the starting species and resulting skeletal mechanisms strongly depend on the local composition in the flames. In addition, the number of retained species may be significant only near the flame front region where chemical reactions are significant. For the one-dimensional methane/air flame considered, speed-up factors of three and five are achieved over the entire simulation for GRI-Mech 3.0 and USC-Mech II, respectively. Greater speed-up factors are expected for larger chemical kinetics mechanisms.

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1. Introduction

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 incorporating detailed chemistry in flame simulations result from the large number of chemical species and the wide range of time scales involved in detailed chemical kinetics [1]. In this study, we consider a reacting ideal gas mixture containing n_s chemical species and composed of n_e elements. The thermochemical state of the mixture at a given location and time is specified by the pressure p , the mixture temperature T , and the vector \mathbf{Y} (length n_s) of species mass fractions.

The governing equations of an inhomogeneous reactive flow can be efficiently solved by numerical schemes based on operator-splitting, which split the governing equations into sub-equations, wherein each subset of equations capture a portion of the physics present in the system. Each subset of equations is integrated separately and sequentially in time to

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advance to the next time step [2–12]. Among the most frequently used splitting schemes is the Strang splitting approach [10], which is second-order accurate in time for sufficiently small time steps.

Operator splitting schemes have been applied to reacting flow simulations. For example, Najm et al. [4] constructed a stiff, operator-splitting projection scheme for the simulation of an unsteady, two-dimensional reacting flow with detailed kinetics. Singer and Pope [8] demonstrated a combined Strang operator-splitting scheme with tabulation for reactive flow simulations with detailed chemical kinetics.

For an adiabatic and isobaric system, with the mathematical equations that govern chemical reactions separated into reaction fractional substeps, the composition vector, $\Phi \equiv \{Y, T\}$, of each computational cell/particle during a single substep evolves according to a set of stiff, nonlinear ordinary differential equations (ODEs),

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

where \mathbf{S} is the rate of change due to chemical reactions. This reaction fractional substep determines the evolution of the thermochemical 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 it may be variable with a typical range spanning several orders of magnitude. When detailed chemical kinetics mechanisms are employed, the major computational challenge of simulating reacting flows within an operator-splitting framework 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 chemical time scales may range from smaller than 10^{-9} s to over 1 s [1].

In the past decade, significant progress has been made in methodologies and algorithms to reduce the computational cost of incorporating detailed chemistry mechanisms into reactive flow simulations. The most widely adopted techniques include, for example, the development of skeletal mechanisms from large detailed mechanisms by the elimination of inconsequential species and reactions [13–19]; dimension-reduction techniques [20–30]; storage/retrieval methodologies [31–36] such as in situ adaptive tabulation (ISAT) [34,35]; cell agglomeration methods such as multi-zone models [37–39]; and dynamic adaptive chemistry (DAC) [40–45]. In particular, the DAC approach [40–45], which reduces computing time by constructing locally (spatially and temporally) valid skeletal mechanisms, has recently gained significant interest.

The DAC approach, which involves on-the-fly reduction of chemical mechanisms, was first proposed by Liang et al. [40] to accelerate the time-integration of Eq. (1). By exploiting the local variation of kinetics sophistication, only a small subset of species and reactions in the full mechanism is required to capture the dominant reaction pathways for specific local conditions over a short time span. Consequently, the ODE system governing chemical kinetics during the reaction fractional step is reduced in size due to the removal of unimportant species. DAC has been successfully demonstrated in internal combustion engine (ICE) simulations [40–43] and general turbulent reactive flow simulations [44,45]. Currently, DAC can be achieved through either the directed relation graph (DRG) method [13,14] or the directed relation graph with error propagation (DRGEP) method [15]. With DAC, no extra memory storage is needed, and the performance of DAC is independent of the combustion system, e.g., steady or unsteady, premixed or non-premixed. The efficiency of DAC increases with mechanism size, and therefore DAC is particularly suitable for combustion simulations with large mechanisms.

In the present study, the combined use of DAC and splitting schemes is applied to reactive flow simulations. Specifically, Strang-based splitting schemes are employed to separate the different physical processes (i.e., transport and chemical reactions) into fractional substeps, and DAC is used to accelerate the calculations of the reaction substeps. The focus of the study is to investigate the effect of DAC on the convergence characteristics of the Strang-based splitting schemes. Consequently, the combined DAC-splitting scheme is applied to one-dimensional, unsteady, freely-propagating, premixed methane/air laminar flames. Other major contributions of the current work include a generalized selection of the starting species in DAC, a detailed error analysis of the reaction substeps when using DAC, and the quantification of the effects of density variations and realistic transport properties on the convergence characteristics of the combined scheme.

An outline of the paper is as follows. In Section 2, the governing equations for the one-dimensional unsteady laminar premixed flame are presented. In Section 3, the Strang-based splitting schemes with DAC for the governing equations are formulated. Computational results are presented in Section 4, which includes an analysis of spatial and temporal convergence, the effect of the DAC reduction threshold on solution accuracy, and the computational savings achieved through DAC. Finally, conclusions are drawn in Section 5.

2. Governing equations

The one-dimensional, unsteady, freely-propagating, laminar premixed flame considered in the present study is adiabatic and isobaric without radiative heat transfer; Soret and Dufour effects are ignored. Therefore, the set of equations governing the system are the conservation of mass, energy, and chemical species:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0, \quad (2)$$

$$\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho u T)}{\partial x} = \frac{1}{c_p} \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{1}{c_p} \sum_{k=1}^{n_s} \dot{\omega}_k h_k W_k, \quad (3)$$

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