Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 36 (2017) 2025–2032

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

Parallel on-the-fly adaptive kinetics in direct numerical simulation of turbulent premixed flame

Suo Yang, Reetesh Ranjan, Vigor Yang, Suresh Menon, Wenting Sun*

School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

Received 3 December 2015; accepted 6 July 2016
Available online 18 July 2016

Abstract

A new numerical framework for direct numerical simulation (DNS) of turbulent combustion is developed employing on-the-fly adaptive kinetics (OAK), correlated transport (CoTran), and a point-implicit ODE solver (ODEPIM). The new framework is tested on a canonical turbulent premixed flame employing a real conventional jet fuel mechanism. The results show that the new framework provides a significant speed-up of kinetics and transport computation, which allows DNS with large kinetic mechanisms, and at the same time maintains high accuracy and good parallel scalability. Detailed diagnostics show that calculation of the chemical source term with ODEPIM is 17 times faster than with a pure implicit solver in this test. OAK utilizes a path flux analysis (PFA) method to reduce the large kinetic mechanism to a smaller size for each location and time step, and it can further speed up the chemical source calculation by 2.7 times in this test. CoTran uses a similar correlation method to make the calculation of mixture-averaged diffusion (MAD) coefficients 72 times faster in this test. Compared to conventional DNS, the total CPU time of the final framework is 20 times faster, kinetics is 46 times faster, and transport is 72 times faster in this test.

Keywords: Turbulent flames; Direct numerical simulation; Reaction kinetics

1. Introduction

The development of 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. Because of high computational cost, DNS and LES typically employ simplified kinetic mechanisms. Oversimplified kinetic mechanisms, however, are known to be of limited functions and may significantly reduce the quality of prediction [1]. Detailed kinetic mechanisms must be considered for accurate prediction, which normally contain a large number of species. In combustion systems, the characteristic timescales can range from millisecond to picosecond or even beyond, so it is prohibitive to use detailed kinetic mechanisms in DNS/LES of turbulent combustion with a large number of grid cells. As a result, chemistry and transport dominate the resource requirements in most combustion DNS studies [2–5].

* Corresponding author.
E-mail address: wenting.sun@aerospace.gatech.edu (W. Sun).

http://dx.doi.org/10.1016/j.proci.2016.07.021
1540-7489

In order to reduce the number of species in detailed kinetic mechanisms, several methods [6–8] have been proposed. While the globally reduced kinetic mechanisms of around 40 species are small enough for most 0D/1D simulations, they are still too large for 3D simulations of turbulent combustion. On the other hand, any further reduction would introduce significant errors, because globally reduced mechanisms typically have to be produced based on conditions of interest in practice. To deal with this issue, several adaptive combustion models have been proposed by a number of investigators. Gou et al. [9] proposed a dynamic adaptive chemistry method with error control for 0D/1D laminar flames, reducing kinetics locally for each grid point and time step. Liang et al. [10] proposed a pre-partitioned adaptive chemistry methodology for 0D partially-stirred reactor using particle probability density function (PDF) methods. In contrast, Wu et al. [11] designed a sub-model assignment framework to assign different flamelet/finite rate sub-models rather than different kinetics to different zones of the simulation domain for a 2D laminar triple flame. This method matches the boundaries of zones by only conserving the interested quantities. Both the on-the-fly reduction and zone partition in all the above methods contain significant CPU overhead for mechanism reduction/zone partition. In order to reduce the CPU overhead, Liang et al. [10] and Wu et al. [11] proposed pre-generating look-up tables for the zone partition. Covering all conditions through tabulation, however, presents challenges, and the large tables make important demands on memory resources. Recently, Sun et al. [12,13] proposed a simple zone-partition criterion to decide whether a new on-the-fly reduction was required or not, and this significantly reduced CPU overhead. Employing the on-the-fly adaptive kinetics (OAK) technique, Sun et al. [12,13] showed significant reduction of CPU time for chemistry in 1D laminar flames.

Molecular diffusion transport modeling is another obstacle to accurate and efficient DNS of turbulent combustion. Bruno et al. [2] compared three models in DNS of a partially premixed flame, and concluded that the mixture-averaged diffusion (MAD) model predicts essentially the same fluid-dynamic and thermo-chemical field as the fully multi-component diffusion (MCD) model, but the fast constant Lewis number model predicts a significantly different flow field. Therefore, the MAD, or a higher fidelity, model is needed to guarantee accurate predictions. Although much faster than the MCD model, applying the MAD model at every time step and every grid cell is still expensive; it is often the 2nd largest component of the CPU time for a given computation, and could dominate CPU use if the kinetic source term is accelerated. To improve the computation of transport properties, Sun and Ju [14] developed a correlated transport (CoTran) technique, and obtained significant further speed-up for extensive 0D/1D laminar flames.

Both the OAK and CoTran techniques have been applied only to 0D and 1D simulations of laminar flames. Generalization of these techniques to 3D DNS of turbulent combustion gives rise to several critical questions: (1) how to efficiently scan and form the correlation zones in 3D space; (2) whether existing CPU overhead reduction methods are adequate for 3D turbulent flames; (3) whether correlation grouping is valid under high intensity turbulence; (4) how to maintain good parallel scaling performance on a large number of processors. In addition, optimized combinations of the above methods to provide the best possible speed have not yet been developed.

In the present work, a new regime-independent framework for 3D DNS of turbulent combustion with detailed kinetics is developed by incorporating on-the-fly adaptive kinetics (OAK), correlated transport (CoTran) techniques, and an efficient point-implicit ODE solver (ODEPIM) into a conventional DNS platform. All three methods are modified and optimized to adapt to 3D turbulent combustion and parallel high performance computing (HPC). The new framework is tested on a canonical premixed flame interacting with decaying isotropic turbulence to evaluate its accuracy, speed-up and parallel performance.

2. Numerical methods

2.1. Reacting flow solver

A well-established numerical flow solver, AVF-LESLIE [15], is employed in this study. It is a multi-physics simulation tool capable of DNS/LES of reacting/non-reacting flows in canonical and moderately complex flow configurations. It has been extensively used in the past to study wide variety of flow conditions, including acoustic flame-vortex interaction, premixed flame turbulence interaction, and scalar mixing [15,16]. It solves the reactive, multi-species, compressible Navier–Stokes equations using a finite-volume-based spatial discretization on generalized curvilinear coordinates. The spatial discretization is based on the well-known 2nd/4th-order accurate MacCormack scheme [17]. The time integration of the semi-discrete system of equations is performed by an explicit 2nd-order accurate scheme. The solver can handle arbitrarily complex finite-rate chemical kinetics and uses double-precision variable-coefficient stiff ODE solver (DVODE) [18]. The thermodynamic properties are computed using a thermally perfect gas formulation, whereas transport properties are obtained through MAD expressions.