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Numerical implementation of mixing and molecular transport in LES/PDF studies of turbulent reacting flows

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ABSTRACT

Probability Density Function (PDF) methods in combination with Large Eddy Simulations (LES) are a powerful tool for studying turbulent reacting flow problems and we are interested in the implementation of mixing and molecular transport in LES/PDF methods. The numerical methodology used for solution procedure is the hybrid particle/mesh method and a fractional step scheme is used to solve for transport, reaction and mixing sequentially. Mixing is modeled using the Interaction by Exchange with the Mean (IEM) model and the effects of molecular transport are incorporated as a mean drift term in the mixing step. This methodology avoids spurious production of scalar variance and also allows direct incorporation of differential diffusion effects. In this study, various numerical implementations of mixing and molecular transport are presented and evaluated, using the Method of Manufactured Solutions (MMS), for (1) accuracy, (2) detailed conservation, (3) realizability, and (4) stability. Moreover, the methodology is shown to be successful in capturing the effects of differential diffusion accurately with the additional property of ensuring realizability of species mass fractions. Finally and most importantly, we describe a new variance reduction technique by way of an implicit smoothing methodology. This smoothing scheme is shown to satisfy conservation, boundedness and regularity criteria. Moreover, for an appropriate choice of the smoothing length scale, significant improvements in accuracy can be achieved for an incremental increase in computational cost. Also, it is shown that with smoothing on a length scale greater than the grid size, the bias and statistical errors due to there being a finite number of particles in the Lagrangian Monte Carlo simulations scale as N_{tot}^{-1} and $N_{tot}^{-1/2}$ respectively, where N_{tot} is the total number of particles in the computational domain, whereas without smoothing these errors scale as N_{pc}^{-1} and $N_{pc}^{-1/2}$, where N_{pc} is the much smaller number of particles in a computational cell.

1. Introduction

The world's energy needs are primarily satisfied by processes that convert the chemical energy stored in the fossil fuels into usable thermal energy. Given the high depletion rate of fuels as compared to the increasing energy needs of growing economies, there is a strong focus on improving the efficiencies of existing facilities by augmenting their designs. Better understanding of the underlying physics behind the turbulent combustion processes inherent in these systems paves a path to designing better systems.

Turbulent combustion involves several species interacting with each other via multiple chemical reactions and with the underlying turbulent flow. Computational fluid dynamics (CFD) based tools [1] have been used to provide various levels of

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description to address the turbulence closure problem [2] encountered in the modeling of turbulent reacting flows. Reynolds Averaged Navier Stokes (RANS) based approaches were historically chosen since the computation of instantaneous flow fields in a turbulent reacting flow was not possible. Given the wide range of temporal and spatial scales inherent in a reacting flow calculation, a DNS (Direct Numerical Simulation) gives the most detailed level of description possible by resolving all scales [3]. On the other hand, a LES (Large Eddy Simulation) resolves only the large scales of the turbulent flow while modeling the effects of the small scales [4–6]. In comparison, DNS is still not computationally tractable for high Reynolds number turbulent flow calculations whereas LES is becoming more commonplace with the development and advancement of high performance computing facilities.

In modeling a turbulent reacting flow, the complexity is magnified multi-fold by large density variations and highly non-linear chemical reaction rates. Probability Density Function (PDF) [4,7–9] methods have been proven to be highly successful in addressing most of the closure problems including closure of the non-linear chemical source terms due to reaction. In the context of LES, based on the filtering operation performed, a PDF analogue called the Filtered Density Function (FDF) [8,10–12] is defined. Though there are many variants to the definition of LES, the most dominant approach is based on 'filtering'. Recently, Pope [13] introduced the idea of self-conditioned fields as an alternative to the filtering approach. In this work, we use the framework based on self-conditioned fields and hence, the terminology PDF instead of FDF.

The present work improves and extends the numerical implementation of LES/PDF methods. Specifically, we present a smoothing technique for spatial averaging of estimated statistics, an evaluation of three numerical implementations of the mixing model with molecular transport and a brief study of the effects of differential diffusion in a simple non-reacting mixing problem.

In a composition-PDF approach, although the effects of reaction appear in closed form and need no modeling, the effects of turbulent transport and molecular mixing need to be modeled. Typically, the effects of turbulent transport are modeled using a gradient diffusion hypothesis. To model the effects of molecular diffusion which appear as a conditional scalar dissipation term in the PDF transport equation, various mixing models have been developed. The Interaction by Exchange with the Mean (IEM) model was postulated in the context of chemical reactor engineering [14]. An identical model called the linear mean-square estimation model (LMSE) was proposed independently by [15]. These models are implemented as being local in physical space for inhomogeneous flows. The Interaction by Exchange with the Conditional Mean (IECM) mixing model [16,17] is designed to be local in velocity space while the Euclidean Minimum Spanning Tree (EMST) mixing model [18] models mixing as being local in composition space. Various other mixing models have been developed such as the MC (Modified Curl) mixing model [19–22] and MMC (Multiple Mapping Conditioning) mixing models [23,24]. In PDF methods, the choice of a mixing model is significant, for instance, to predict local extinction in Sandia flames E and F [25]. However, recent studies have shown that in LES/PDF methods, the subgrid-scale mixing closure provided by the IEM mixing model is adequate in most practical situations [26]. Therefore, in the current work, we employ the IEM mixing model to close the conditional dissipation term in the PDF transport equation.

The modeled PDF transport equation is solved using Lagrangian Monte Carlo particle methods. One of the initial works that established a formal relationship between particle models and PDF methods was by Pope [27]. The Lagrangian particle methods associated with the PDF transport in the form in use today are based on Pope's 1985 paper [7]. Here, the turbulent flow is represented by a large number of notional particles, all of which are considered to be statistically independent. Models are constructed to evolve the properties of the particles in time. The resulting stochastic differential equations (SDE) are solved to account for particle transport, mixing and reaction. Solving for the evolution of these particles corresponds to the solution of the modeled PDF transport equation. The first use of this approach to LES/PDF is due to Colucci et al. [11].

The conditional diffusion term in the PDF transport equation represents both molecular transport in physical space and molecular mixing in composition space. In most previous studies, the effects of molecular transport are incorporated as a random walk term in the particle transport equation, as first proposed by Anand and Pope [28]. Recently, McDermott and Pope [29] show that modeling the effects of molecular transport as a random walk in the particle position equation results in a spurious production of scalar variance in the DNS limit. They propose an alternative approach to modeling molecular transport as a mean drift term in the particle scalar evolution equation, and this avoids the spurious production of variance. LES studies of a laboratory-scale turbulent flame (Sandia flame D) [30] also show that on reasonably resolved grids, the molecular diffusivity is dominant as compared to the subgrid turbulent diffusivity in the near-field of the jet, indicating that the effects of molecular transport need to be treated accurately in LES/PDF models of turbulent reacting flows.

The current work is based on the models and algorithms implemented in the HPDF code described by Wang and Pope [31]. Micro-mixing is modeled using the IEM mixing model and the effects of molecular transport are modeled as a mean drift term as mentioned above [29]. This modeling strategy has the additional advantage of being able to account for the effects of differential diffusion. The mixing model is implemented such that problems of interest in both Cartesian and cylindrical coordinate systems can be effectively handled. We also require that the numerical schemes used to implement mixing satisfy the following criteria: (1) they satisfy detailed scalar conservation, (2) they ensure realizability, (3) they are stable and (4) they are accurate.

A typical PDF calculation of a turbulent reacting flow is performed with a nominal number, N_{pc}, of 20–50 particles per finite volume cell. In order to maintain an acceptable distribution of particles in space, various particle number control algorithms are used [9,32]. The numerical errors associated with a hybrid particle/mesh methodology can be classified broadly into statistical error, bias error, spatial truncation error and temporal discretization error. Among these, the statistical error is of random nature while the latter three are deterministic and cannot be reduced by averaging. The statistical error scales as