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A minimally-dissipative low-Mach number solver for complex reacting flows in OpenFOAM

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ABSTRACT

Large eddy simulation (LES) has become the de-facto computational tool for modeling complex reacting flows, especially in gas turbine applications. However, readily usable general-purpose LES codes for complex geometries are typically academic or proprietary/commercial in nature. The objective of this work is to develop and disseminate an open source LES tool for low-Mach number turbulent combustion using the OpenFOAM framework. In particular, a collocated-mesh approach suited for unstructured grid formulation is provided. Unlike other fluid dynamics models, LES accuracy is intricately linked to so-called primary and secondary conservation properties of the numerical discretization schemes. This implies that although the solver only evolves equations for mass, momentum, and energy, the implied discrete equation for kinetic energy (square of velocity) should be minimally-dissipative. Here, a specific spatial and temporal discretization is imposed such that this kinetic energy dissipation is minimized. The method is demonstrated using manufactured solutions approach on regular and skewed meshes for a canonical flow and a lab-scale turbulent flow problem.

1. Introduction

The use of large eddy simulation in complex turbulent flows has increased substantially in the last decade. This advance is being driven by the rapid growth in computational power, as well as advances in numerical algorithms for such complex flows. This has led to the development of a number of LES solvers that are routinely deployed in industrial applications [1–5]. Nevertheless, many of these solvers remain proprietary and not open to the research community. This deficiency is particularly challenging for LES due to the sensitivity of LES results to numerical accuracy. For instance, when head-to-head comparison of LES models are made, such studies rely on different LES solvers and numerical methods. Consequently, the conclusions are highly sensitive to these numerical details, and may not even be relevant to model comparison [6]. Furthermore, many combustion models and subfilter closures are developed for canonical flow problems and are not exercised in full-scale geometries or application-relevant flow problems. This sparsity in full-scale validation is at least partially due to the lack of an easy approach to porting models to complex flow problems. As LES models mature, there is a clear need for a robust open source platform to demonstrate their performance for practical configurations. In this context, OpenFOAM [4] is a prime candidate for such a framework. Based on a field operation approach [7], OpenFOAM provides a convenient code-base for numerically solving partial differential equations. Moreover, OpenFOAM has developed a broad community of developers and users, who have added valuable tools and methods to the base solver [8]. This robust development ecosystem has been leveraged extensively in the turbulent flow and turbulent combustion research and application communities [9–12]. The current work intends to upgrade the implementation of LES algorithms that are indispensable in solving variable density reacting flows of interest to gas turbine applications. With the will of gradually moving combustion research applications to OpenFOAM, key issues regarding LES numerical accuracy are addressed.

Many gas turbine applications, especially related to the combustor section, operate in the low-Mach number regime, characterized by velocities smaller than 0.3 Ma, where the Mach number is defined based on local fluid properties. In this regime, the acoustic component of the Navier-Stokes equations is decoupled from the basic flow physics. Consequently, by reformulating the governing equations for this low-Ma regime, it is possible to go beyond

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the CFL restriction imposed by the acoustic wave speed (i.e., local sound speed). In many applications, this can amount to an order of magnitude increase in timestep used. Although OpenFOAM has been used for combustion applications, many of these are related to the compressible flow regime (see, for instance Ref. [10]). In the base distribution of OpenFOAM, the variable density solver the closest to a low-Mach number solver uses an all-Mach approach, where some level of compressibility-related coupling of the governing equations is retained even in the limit of zero Mach number [13]. Hence, developing a robust low-Ma solver for variable density flows will be of interest to combustion applications.

Another issue of importance to LES is the coupling between numerical discretization and modeling errors, as discussed in [14–19]. Briefly, there are two types of numerical errors. First, the spatial discretization of derivative operators for fields containing high wave number components can be highly erroneous [20]. In practical LES, features comparable to the filter size can thus be contaminated by discretization errors [14,18,21]. In turbulent combustion applications, where small-scale models are critical for capturing the mixing and reactions processes, this discretization error represents a major concern. The most comprehensive solution is to use an explicit filtering technique, where the small-scales are removed through a filter during the simulation in order to prevent deposition of energy at such scales [14,15,22,23]. However, extending these techniques to variable density flows has not been achieved yet [24]. Several approaches [19,25] have been proposed to mitigate these numerical effects. The second issue concerns the so-called conservation of secondary quantities. Finite-volume approaches discretely conserve primary quantities such as mass and momentum. With LES, the accurate representation of the turbulent energy spectrum is important for the validity of the modeling assumptions. Therefore, minimizing numerical dissipation of kinetic energy is a key point of the LES solvers. In low-Mach number incompressible flows, and in the absence of viscous dissipation, kinetic energy should be exactly conserved. In this case, the spatial and temporal discretization should ensure that such conservation or, at the least, a minimization of dissipation is achieved [13]. In this regard, there has been considerable progress in the design of energy-conserving numerical schemes [26–30]. Again, a comprehensive implementation of such tools in the OpenFOAM framework is not available.

With this introduction, the objectives of this work are as follows: 1) Analyze the variable density solvers in OpenFOAM, and implement a consistent low-Ma solver that preserves spatial and temporal accuracy in the limit of zero Mach number, and 2) evaluate the energy conserving properties of existing OpenFOAM solvers, and implement a minimally-dissipative approach. In Section 2, based on existing schemes, a strict variable density low-Mach number solver is designed and its implementation in OpenFOAM is described. The solver is then tested using the method of manufactured solutions. Section 3 provides the necessary theoretical background for the design of energy conservative solvers. In Section 4, the implementation of a minimally-dissipative solver is described for the OpenFOAM framework. Finally in Section 5, a set of verification and validation cases are used to demonstrate the capabilities of the new solver. As will be discussed below, the key approaches are derived from existing algorithms, but the choice of discretization schemes and solution methods is unique and is shown to be necessary for a generic open source solver, such as the one used here.

2. Low-Mach number solvers in OpenFOAM

The governing equations of fluid flow of interest here are written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{1}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \overline{\boldsymbol{\sigma}}, \tag{2}$$

where ρ is the flow density, $\boldsymbol{u}$ is the local gas phase velocity vector, p is the mechanical pressure and $\overline{\boldsymbol{\sigma}}$ is the viscous stress tensor.

When considering chemical reactions, additional equations that describe transport of chemical species and a formulation that couples any heat addition to the density term need to be included. A generic scalar transport equation that may be used for this purpose is given by:

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \boldsymbol{u}) = \nabla \cdot (D \nabla \phi) + \dot{\omega}, \tag{3}$$

where ϕ denotes the transported scalar and D denotes mass diffusivity and $\dot{\omega}$ is some volumetric source term.

To solve this system of equations, a numerical approach is used. Three different types of flow solvers are defined here for the sake of future discussion. An *incompressible solver* is defined as a solver that does not take into account any density change. In other words, the density field is treated as a constant value. A *compressible solver* is defined as a solver that takes into account the dynamic coupling between the pressure and density fields. In other words, this solver allows mechanical energy (kinetic energy noted KE) to be converted to thermal energy (through pressure). A *low-Mach number solver* is defined as a solver that does not couple density changes with instantaneous pressure changes. In particular, the pressure field is split into a thermodynamic pressure and a mechanical pressure, with the former held constant while the latter is allowed to vary through velocity changes in the flow. The thermodynamic pressure is used in the equation of state, while the mechanical pressure appears in the momentum transport equation (Eq. (2)). Density variations in low-Mach number solvers occur through heat addition or removal, for instance due to chemical reactions. Such low-Ma number flows and associated solvers are the focus of this work.

2.1. Hybrid solvers in OpenFOAM for variable density flows

The base distribution of OpenFOAM [4] contains a suite of solvers targeting reacting flows that involve density changes. Although they nominally fall under the compressible solver definition provided above, some aspects of the low-Mach representation is also included. The main choice is as follows: all variable density solvers use the equation of state to reduce the number of partial differential equations needed (for the thermochemical part) to two of the three variables (pressure, temperature, density). Assuming that an energy equation that provides temperature is available, the choice is then to solve for density and obtain pressure from equation of state or vice-versa. These two types of compressible solvers are: the *density-based solvers* where the density is transported using the continuity equation, and the *pressure-based solvers* where the thermodynamical pressure is computed using a pressure correction method. In the pressure-based solvers handling variable density available in OpenFOAM, a generic pressure correction procedure [13, Ch. 10.2] is used. This approach is easily applicable even with unstructured and complex grids. The pressure correction equation contains an incompressible divergence term (correcting the mass fluxes) and a compressible convective term (correcting the density). Each one of these term becomes dominant when the flow is largely incompressible or compressible, respectively. This pressure-correction strategy is referred to as a *hybrid* approach in the remainder of the paper. This type of pressure correction has been used to simulate combustion cases at high and low-Mach numbers [9,31].

Since the pressure correction has an impact on the density field, this procedure involving momentum, scalar transport and pressure