Journal of Computational Physics 274 (2014) 413–431

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A velocity divergence constraint for large-eddy simulation of low-Mach flows

Randall J. McDermott

Fire Research Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

ARTICLE INFO

Article history:
Received 29 August 2013
Received in revised form 28 May 2014
Accepted 11 June 2014
Available online 17 June 2014

Keywords:
Large-eddy simulation
LES
Low-Mach flow
Projection scheme
Divergence constraint

ABSTRACT

The velocity divergence (rate of fluid volumetric expansion) is a flow field quantity of fundamental importance in low-Mach flows. It directly affects the local mass density and therefore the local temperature through the equation of state. In this paper, starting from the conservative form of the sensible enthalpy transport equation, we derive a discrete divergence constraint for use in large-eddy simulation (LES) of low-Mach flows. The result accounts for numerical transport of mass and energy, which is difficult to eliminate in relatively coarse, engineering LES calculations when total variation diminishing (TVD) scalar transport schemes are employed. Without the correction terms derived here, unresolved (numerical) mixing of gas species with different heat capacities or molecular weights may lead to erroneous mixture temperatures and ultimately to an imbalance in the energy budget. The new formulation is implemented in a publicly available LES code called the Fire Dynamics Simulator (FDS). Accuracy of the flow solver for transport is demonstrated using the method of manufactured solutions. The conservation properties of the present scheme are demonstrated on two simple energy budget test cases, one involving a small fire in a compartment with natural ventilation and another involving mixing of two gases with different thermal properties.

Published by Elsevier Inc.

1. Introduction

In this paper, starting from the conservative form of the sensible enthalpy transport equation, we derive a numerically consistent velocity divergence constraint for use in large-eddy simulation (LES) of low-Mach flows. The result accounts for numerical transport of mass and energy, which is difficult to eliminate in relatively coarse, engineering LES calculations when total variation diminishing (TVD) scalar transport schemes are employed. Without the correction terms derived here, unresolved (numerical) mixing of gas species with different heat capacities or molecular weights may lead to erroneous mixture temperatures and ultimately to an imbalance in the energy budget.

Equations describing low-speed, variable density flows were derived by Rehm and Baum in 1978 [1] to model thermally-driven buoyant plumes. This system of equations has since been extended to include viscous flows [2,3] and is the basis for many prominent turbulent reacting flow solvers, e.g., [4–8]. Applications suitable to the low-Mach approximation include, but are not limited to, modeling atmospheric pollutant dispersion, gas turbine engines, thermo-nuclear flames, and fire. The author is among the principal developers of a low-Mach LES code called the Fire Dynamics Simulator (FDS) [9], used

E-mail address: randall.mcdermott@nist.gov.

http://dx.doi.org/10.1016/j.jcp.2014.06.019
0021-9991/Published by Elsevier Inc.

primarily for building design and safety analysis by fire protection engineers, but also used in forensic reconstruction of fire events [10].

For chemically reacting flows involving heat release, achieving consistent coupling between the species mass fractions, the mass density, the energy, and the equation of state within a time-marching algorithm is nontrivial. Often, iterative methods are employed to find consistent solutions [4,5,7]. The "EKT" ("echt konservativer transport", "fully conservative transport" in German) algorithm of Kempf [6] is an exception. The present work, which differs from EKT in several important respects, introduces a consistent *explicit* scheme which satisfies the conservative form of the mass, species, and energy transport equations.

The FDS formulation is most closely related to the low-Mach formulation of Bell [4] who uses an approximate projection [11] on a collocated grid to satisfy a thermodynamic velocity divergence constraint. This constraint is derived by factoring the divergence out of the continuity equation, substituting the ideal gas equation of state (EOS) for density, and then differentiating the EOS. Bell then solves a conservative enthalpy equation and iterates until the temperature obtained from the enthalpy and the EOS are consistent. In contrast, FDS employs an exact projection on a staggered grid [12], explicitly solves the continuity equation for mass density, factors the divergence from the enthalpy equation, and obtains temperature from the EOS. At this stage in the FDS algorithm, as the analysis in this paper shows, the temperature may not be consistent with a conservative solution of the enthalpy equation unless careful consideration is given to the effects of numerical mixing.

The mixing corrections derived here for the velocity divergence—which prevent First Law (energy conservation) violations in the FDS algorithm—are reminiscent of flux corrections needed to satisfy the *entropy condition* for compressible finite-volume methods [13–17]. The issue of flux accuracy, however, is separate from the issue addressed in this paper. In any practical combustion simulation we are likely to encounter scalar discontinuities, such as the interface between fuel and oxygen in a diffusion flame (we cannot resolve a flame front in LES), where the flux accuracy must degrade to first order by Godunov's theorem. For a numerical scheme to conserve both mass and energy in such cases, with a consistent velocity field, the divergence corrections derived here must be incorporated, either explicitly into the divergence constraint (which we argue is the most efficient approach) or implicitly through iteration of the mass, momentum, and energy solutions. *The key result of this paper is recognition that the discretization of the state variables (enthalpy and composition) may be inconsistent with the assumed variation of the thermodynamic pressure (the key assumption in the low-Mach formulation) unless the proper corrections are employed (either explicitly or through iteration).* Note that compressible formulations do not suffer this problem because the thermodynamic pressure may vary locally in tight concert with the equation of state.

Furthermore, in low-Mach LES formulations it is common to use kinetic-energy-preserving spatial discretizations for the momentum equation [5,18–21]. In short, central differences are employed for momentum while TVD schemes are typically employed for scalars. This allows kinetic energy to be preserved in the absence of physical viscosity (assuming the time discretization is suitable) and subgrid models for the turbulent stress become wholly responsible for the leading-order physics of transferring kinetic energy from the resolved scales to the unresolved scales of motion (that is, dissipating kinetic energy from the grid). But, regardless of the conservation properties of the spatial discretizations, the time marching scheme—in which the divergence constraint plays a key role for low-Mach flows—is ultimately responsible for maintaining consistency between mass, momentum, (thermal) energy, and the equation of state.

The remainder of this paper is organized as follows. Next, in Section 2, we outline the mathematical formulation drawing attention to the role played by the velocity divergence. In Section 3, we derive the divergence constraint, which is the main focus of this work. Test cases illustrating accuracy of the flow solver, the potential energy imbalance, and the effect of numerical mixing are presented in Section 4. This is followed by a discussion in Section 5 of the correction terms and a viable simplification to the divergence constraint which avoids the need for the corrections. Finally, conclusions are stated in Section 6.

2. Governing equations

Filtering The equations for large-eddy simulation (LES) are derived by applying a low-pass filter, parameterized by a width Δ, to the transport equations for mass, momentum, and energy. For our purposes, it is sufficient to think of the filtered fields in the LES equations as cell means. For example, in one dimension the filtered density, $\bar{\rho}(x,t)$, is

$$\bar{\rho}(x,t) = \frac{1}{\Delta} \int_{x-\Delta/2}^{x+\Delta/2} \rho(r,t)\, \mathrm{d}r. \tag{1}$$

In FDS, the filter width, Δ, is equivalent to the local cell size, Δx, and is a key parameter in the submodels for the turbulent viscosity and the reaction time scale, discussed later. In what follows, the filter formalism is relaxed (the overline notation is suppressed for readability) since no explicit filtering operations are performed in the algorithm.

Low-Mach formulation In the low-Mach formulation, the pressure is decomposed into a background thermodynamic pressure (used in the equation of state) and a fluctuating hydrodynamic pressure (which drives local fluctuations in the flow field),