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Explicitly-filtered LES for the grid-spacing-independent and discretization-order-independent prediction of a conserved scalar

Senthilkumaran Radhakrishnan, Josette Bellan *

Jet Propulsion Laboratory, California Institute of Technology, CA 91109, United States

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ABSTRACT

The previously proposed methodology of Explicitly Filtered Large Eddy Simulation (EFLES) predicts velocity fields that are grid-spacing and discretization-order independent for single-phase, and for two-phase compressible flows. In the current study, EFLES is tested for determining the predictability of a passive scalar evolution in turbulent flows, and the EFLES results are also compared to equivalent ones obtained with conventional Large Eddy Simulation (LES). A single Direct Numerical Simulation (DNS) realization of a temporal mixing layer is conducted with an initial Reynolds number of 1800. After an initial transient, the mixing-layer momentum thickness grows linearly with time. The DNS is continued during the linear growth period and until the momentum thickness Reynolds number reaches 6405. The filtered and coarsened DNS (FDNS) database is considered the template to be reached by LES or EFLES. Both LES and EFLES are conducted using the dynamic Smagorinsky model. Three grids – coarse, medium and fine – and three discretization orders – fourth, sixth and eighth – are used for each LES and EFLES. In contrast to conventional LES where the grid spacing and the filter width are proportionally related, in EFLES the filter width is set beforehand and independent of the grid spacing. The criteria for comparing LES and EFLES results to the FDNS encompass both averages and second-order quantities that characterize the passive scalar behavior. Homogeneous plane averages combined with time averaging past the time when the mixing layer becomes turbulent, enabled the computation of smooth statistics for comparison between FDNS and LES or EFLES. It is found that the conventional LES results are not predictive in that refining the grid or increasing the discretization order, or both, does not lead to coincidence of the results. In contrast, refining the grid past the medium spacing for the sixth- and eighth-order discretizations leads to the EFLES results collapsing on a single curve. Thus, the medium grid spacing and sixth discretization order is the most computationally economic predictive simulation. Based on these findings, EFLES computations, the predictions of which are unaffected by numerical errors, are recommended for model validation with experimental data.

1. Introduction

The prediction of a conserved scalar is important in many fields of study. For example, in modeling of combustion processes, if a conserved scalar exists, the mathematical problem can be greatly simplified (e.g. a conserved scalar may not exist in species mixtures in which there is differential diffusion among species); the flamelet model [1] judiciously takes advantage of the possible existence of a conserved scalar to substantially reduce the complexity of turbulent flame modeling when flames are thinner than the Kolmogorov scale. Inert gases transported in mixtures of other gases are also simulated by a conserved scalar. The motion of particles with negligible inertia and smaller than the Kolmogorov scale can also be described using a passive scalar approach. Thus, this concept is also applicable to atmospheric sciences where pollutant dispersion can be studied by using a passive scalar approach. Similarly, in oceanography, contaminant and nutrient transport can be studied using a passive scalar approach.

Despite the substantial importance of conserved scalars, the predictive capability for their behavior in turbulent flows is hampered by the fact that the most popular methods for turbulent flow simulations are either not accurate, or not grid-spacing and discretization-order independent, or both. For example, the Reynolds Average Navier Stokes (RANS) method [2] can be made grid-spacing independent by successively refining the grid until the results from the refinements coincide; but because of its inherent construct, RANS can only predict averages rather than detailed

* Corresponding author. Tel.: +1 818 354 6959; fax: +1 818 393 6682.
E-mail address: josette.bellan@jpl.nasa.gov (J. Bellan).

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behavior. At the other extreme is the conventional Large Eddy Simulation (LES) [2] in which the scales larger than a filter width are resolved and those smaller than the filter width are modeled using Subgrid Scale (SGS) models. These SGS models compute the contribution of the small scales using the solution at the larger scales that itself depends on the grid spacing. Because in LES, the SGS model is dependent on the grid spacing, a typical grid refinement study does not lead to a grid converged solution.

Using an explicit filter to remove those scales which may have been contaminated by numerical errors has been employed in the past ([3,4]) and the methodology was called Explicitly-Filtered Large Eddy Simulation (EFLES). In fact, the idea of explicit filtering predates these more recent studies (e.g. [5,7,6,8,9]), but in most previous investigations the goal was different from obtaining grid-independent solutions: e.g. in Ref. [7] explicit filtering was used to control the impact of numerical errors and also compared it with utilizing mesh refinement to increase simulation accuracy, while in Ref. [6] the larger accuracy in predicting turbulence intensities was noted when using explicit filtering together with a reconstruction of the SGS scales. Only in Ref. [9] was the issue of grid-spacing independence addressed for an incompressible channel flow. The study of Radhakrishnan and Bellan [3] showed that modifying the conventional LES formulation by explicitly filtering in the conservation equations the non-linear terms which substantially produce small scales, and by uncoupling the filter width from the LES-grid spacing, one can achieve both grid-spacing and discretization-order independence for predicting the velocity field in compressible turbulent flow. Using EFLES for drop-laden flows, Radhakrishnan and Bellan [4] have investigated some properties of a non-conserved scalar (i.e. the partial density of the vapor emanating from the drops) and found that they are also grid-spacing and discretization-order independent.

Several concepts are of importance in simulations of turbulent flows: the smallest scale of interest to the modeler at which the solution should be computed; the predictability of the code defined as the ability to provide the same results, independent of the numerical aspects (i.e. grid spacing and discretization order), for a given set of inputs, in effect eliminating the impact of numerical aspects on the solution; and the accuracy of the simulation defined as the ability to agree with a template, an aspect which is determined by the SGS models replacing the information filtered below the scale of interest. Clearly, the modeler must first choose the smallest scale of interest before predictability or accuracy can be considered; this is in effect the filter width. Therefore, the filter width is an independent parameter in LES or EFLES, in addition to the grid-spacing and the SGS models that also depend on the choice of the filter width. In our view, the attribute of predictability takes higher precedence over that of accuracy in the sense that predictability must be achieved first, before accuracy can be evaluated. Without predictability there is no way to judge accuracy since the results will then depend on the grid spacing. For example, if a LES model is evaluated with data, when the same LES is used in absence of data (which is the situation where LES would have practical value) there is no certainty that the same grid spacing will be used as in the test with the data since the conditions of the study will be different. Because the result of LES is grid-spacing dependent, the conclusions regarding accuracy reached from the evaluation with data may be entirely irrelevant for the practical application since LES is grid-spacing dependent.

Here, we wish to present an in-depth investigation of a conserved scalar and the study is performed for a Reynolds number larger than that considered in Ref. [4]. In Section 2, we present the governing equations which are solved using Direct Numerical Simulation (DNS); the filtered and coarsened (to the LES grid spacing) database, FDNS, represents our template for the LES/EFLES predictions. Each of the LES and EFLES formulations are mathematically described in section 3. The mixing layer configuration, and the initial and boundary conditions are discussed in Section 4, followed by Section 5 in which we explain the numerical methodology. The results are presented in Section 6, and conclusions are offered in Section 7.

2. Governing equations for Direct Numerical Simulation

The situation addressed here is that of a subsonic flow of a perfect gas with constant specific heats, obeying Newtonian constitutive laws.

Following Ref. [10], we define the vector of gas-phase conservative variables $\phi = \{\rho, \rho u_i, \rho e_t, \rho Y\}$ which represents the flow field, with ρ, u_i, e_t and Y respectively being the density, the velocity in the x_i coordinate direction, the total energy and the mass fraction of a passive scalar. The set of conservation equations is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2}$$

$$\frac{\partial(\rho e_t)}{\partial t} + \frac{\partial(\rho e_t u_j)}{\partial x_j} = -\frac{\partial(p u_j)}{\partial x_j} - \frac{\partial q_j}{\partial x_j} + \frac{\partial(\sigma_{ij} u_i)}{\partial x_j}, \tag{3}$$

$$\frac{\partial(\rho Y)}{\partial t} + \frac{\partial(\rho Y u_j)}{\partial x_j} = -\frac{\partial j_j}{\partial x_j}. \tag{4}$$

The internal energy, e is computed as $e = e_t - e_k$, where $e_k = u_i u_i/2$ is the kinetic energy, and the pressure, p, is computed from the prefect gas equation of state

$$p(\phi) = \rho R(\phi) T(\phi), \tag{5}$$

where $R(\phi) = R_u/m, R_u$ is the universal gas constant and m is the molar mass of the gas, and T is the temperature computed from e as

$$e(\phi) = C_v(\phi) T(\phi), \tag{6}$$

where C_v is the mixture heat capacity at constant T. The enthalpy, $h = e + p/\rho$ is computed as

$$h(\phi) = C_p(\phi) T(\phi), \tag{7}$$

where $C_p(\phi)$is the heat capacity at constant p ($C_p = C_v + R$).

The viscous stress, σ_{ij}, in Eqs. (1)–(4) is defined as

$$\sigma_{ij}(\phi) = 2\mu\left(S_{ij} - \frac{1}{3} S_{kk}\delta_{ij}\right), \tag{8}$$

$$S_{ij}(\phi) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{9}$$

where S_{ij} is the rate of strain and μ is the viscosity. The passive-scalar mass flux is computed from

$$j_j(\phi) = -\rho D \frac{\partial Y}{\partial x_j}, \tag{10}$$

where D is the diffusion coefficient, and the heat flux is

$$q_j(\phi) = -\lambda \frac{\partial T(\phi)}{\partial x_j}, \tag{11}$$

where λ is the thermal conductivity. All coefficients μ, D and λ are assumed constant, and they are related through the Prandtl and Schmidt numbers, $Pr = \mu C_p/\lambda$ and $Sc = \mu/(\rho D)$.

3. Large Eddy Simulation formulations

The essential characteristic of LES is that the large-scale contribution of the flow field is obtained by filtering the governing equations. The filtering operation is defined as