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Mixing, scalar boundedness, and numerical dissipation in large-eddy simulations

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ABSTRACT

Numerical schemes for scalar transport and mixing in turbulent flows must be high-order accurate, and observe conservation and boundedness constraints. Discretization accuracy can be evaluated from the truncation error, and assessed by its dispersion and dissipation properties. Dispersion errors can cause violation of physical scalar bounds, whereas numerical dissipation is key to mitigating those violations. Numerical dissipation primarily alters the energy at small scales that are critical to turbulent mixing. Influence of additional dissipation on scalar mixing in large-eddy simulations (LES) of incompressible temporally evolving shear flow is examined in terms of the resolved passive-scalar field, $\bar{Z}$. Scalar fields in flows with different mixing behavior, exhibiting both uniform and non-uniform mixed-fluid composition across a shear layer, are compared for different grid resolutions, subgrid-scale models, and scalar-convection schemes. Scalar mixing is assessed based on resolved passive scalar probability density function (PDF), variance, and spectra. The numerical-dissipation influence on mixing is found to depend on the nature of the flow. Mixing metrics sensitive to numerical dissipation are applied to examine the performance of limiting methods employed to mitigate unphysical scalar excursions. Two approaches, using a linear-scaling limiter for finite-volume schemes and a monotonicity-preserving limiter for finite-difference schemes, are studied. Their performance with respect to accuracy, conservation, and boundedness is discussed.

1. Introduction

Passive or active scalar transport and mixing by turbulent flow is important in numerous engineering and scientific applications (e.g., [1–3] and references therein). Grid-resolution requirements and the resulting computational cost of simulations of high Reynolds- and Schmidt-number flows, where a wide range of spatial and temporal scales determine scalar mixing, place a direct calculation of all scales out of reach. Moreover, for high Schmidt numbers (Sc), the Batchelor scale ($\eta_B \simeq \eta\, Sc^{-\frac{1}{2}}$) is smaller than the Kolmogorov scale (η), and a finer grid is required to fully resolve the scalar field than the velocity field. Large-eddy simulations (LES) lower the computational cost by modeling dynamic effects, on the resolved flow field, of spatial scales smaller than a cutoff wavenumber, while directly calculating the larger scales of motions [4,5]. However, such modeling introduces subgrid-model errors in addition to numerical-discretization errors. Model errors are difficult to quantify without a corresponding direct numerical simulation (DNS) solution, which is usually out of reach for

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practical problems of engineering interest. Therefore, analyses of the interaction between the model and numerical errors are typically restricted to canonical flows at low to moderate Reynolds number [6–9]. Several studies have examined the role of the filter-grid ratio $\Delta/\Delta x$ [8,10–12], where Δ is the filter width and Δx is the grid spacing, and the discretization of the non-linear term [13,14] in LES to keep numerical errors smaller than subgrid-scale (SGS) model contributions. These references and others (e.g., [15,16]) study effects of LES model and numerical errors on the velocity field. In this work, effects of numerical-dissipation errors on a convected passive-scalar field, specifically on scalar boundedness and resolved and subgrid scalar-mixing estimates, are examined.

For uniform-density and uniform-diffusivity flow, the passive-scalar field, Z, is governed by the advection–diffusion equation

$$\frac{\partial Z}{\partial t} + u_j \frac{\partial Z}{\partial x_j} = \mathcal{D} \frac{\partial^2 Z}{\partial x_j^2}, \tag{1}$$

where u_j is the velocity and $\mathcal{D}$ denotes the diffusivity, here assumed to be uniform in space. Solutions to (1) obey the maximum principle, i.e., solution extrema can only occur at the (spatial or temporal) boundary, bounding Z by its initial and boundary values.

In practice, numerical solutions to (1) obtained from a high-order finite-difference/-volume method incur dispersion errors that may result in violations of the maximum principle. The high-wavenumber content of the solution is more susceptible to dispersion (phase-speed) errors, which are of concern to LES since such calculations are, by definition, under-resolved with higher energies at grid scale than if the flow were fully resolved.

If the SGS model does not provide adequate dissipation for a sufficiently smooth scalar field, dispersive oscillations can produce unphysical scalar excursions [17]. These excursions are commonly mitigated using upwind schemes [18,19], or bound-preserving limiters [20,21], both of which introduce artificial dissipation and can lower the accuracy of numerical solutions.

In this study, our aim is two-fold: (1) Examine the effect of numerical dissipation on mixed-fluid composition and scalar fluctuations in different mixing regimes of turbulent shear flows to identify flow statistics sensitive to additional dissipation. Mixed-fluid composition is assessed from scalar PDFs whereas scalar fluctuations from their second central moment, the variance. (2) Use flow statistics sensitive to additional dissipation to assess the numerical dissipation introduced by two limiting procedures, using the linear-scaling limiter of [22,23] and the monotonicity-preserving limiter of [24], to enforce scalar boundedness.

From among the desirable properties of high-order accuracy, conservation, and boundedness, numerical schemes generally satisfy the former two properties but do not strictly impose the third. To enforce scalar boundedness, commonly-used approaches compromise either accuracy, for example with bound-preserving low-order schemes [18,19,21], or conservation, with semi-Lagrangian schemes employing bounded interpolation [20]. In this work, limiting approaches for incompressible-flow simulations that ensure scalar boundedness and conservation while preserving uniform high-order accuracy are discussed.

Liu & Osher [22] developed a linear-scaling limiter for scalar-conservation laws that was adapted to ensure boundedness with uniform high-order accuracy by Zhang & Shu [23] for finite-volume and discontinuous-Galerkin discretizations. The limiter was used in combination with a first-order scheme by Subbareddy et al. [21] to mitigate scalar excursions in compressible-flow simulations with finite-volume schemes. For incompressible-flow computations, a velocity reconstruction consistent with the incompressibility condition ensures boundedness without the need of incorporating a low-order scheme, thus ensuring a uniform high-order accuracy. Such reconstructions are shown in this paper for a velocity field calculated from the non-dissipative schemes of Morinishi et al. [25]. However, the limiting approach of [22,23] cannot be applied to finite-difference schemes, which led us to explore the application of the monotonicity-preserving limiter of Suresh & Huynh [24] to enforce scalar boundedness with finite-difference schemes. Numerical dissipation introduced by each methodology is assessed based on scalar-mixing estimates in a canonical turbulent shear flow.

In Section 2.1, the LES governing equations and the SGS models used in this study are discussed. The evolution of scalar fields with initial conditions leading to different mixing behavior in the temporally evolving shear flow is discussed in Section 2.2. Limiting approaches to mitigate unphysical scalar excursions in incompressible-flow simulations are discussed in Section 3. Several convection schemes with different dissipation and boundedness properties are examined and listed in Section 4.1 along with their global scalar-excursion statistics. The effect of numerical-dissipation errors on scalar-mixing estimates is examined in Section 4.2. Scalar boundedness and numerical dissipation introduced by the limiting methodologies of Section 3 is assessed in Section 4.3.

2. Flow description

2.1. Governing equations and SGS models

For LES, the conservation equations are assumed to be spatially filtered using a kernel $G(\mathbf{x}; \Delta)$, where Δ is the filter width, and a filtered (or resolved) quantity $\bar{f}(\mathbf{x}, t)$ is obtained by convolution of $f(\mathbf{x}, t)$ with $G(\mathbf{x}; \Delta)$ [26]. An explicit convolution calculation is computationally expensive [11] and, in practice, the computational grid typically serves as the spatial