Investigation of turbulence model and numerical scheme combinations for practical finite-volume large eddy simulations

Adetokunbo A. Adedoyin, D. Keith Walters, and Shanti Bhushan

Department of Mechanical Engineering, Mississippi State University, Starkville, USA; Center for Advanced Vehicular Systems, Mississippi State University, Starkville, USA

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Large eddy simulation (LES) is known to suffer from two primary error sources – the subgrid stress (SGS) model and the numerical discretization scheme. These cannot be separately quantified for finite-volume numerical simulations, but an appropriate combination can yield ‘engineering accurate’ prediction of turbulence dynamics. This paper seeks to evaluate combinations of commonly used second-order numerical schemes and Smagorinsky-type SGS models for practical LES. Error assessments are performed for isotropic decaying turbulence using both pseudospectral and finite-volume solvers, followed by validation for a complex turbulent flow of engineering interest. Error assessment using pseudospectral techniques is performed to isolate finite-differencing and modeling errors by explicitly adding numerical derivative error terms to the simulations. Error assessment using the finite-volume method focuses on identification of optimal model-discretization combinations for the best LES predictions using application solvers. The pseudospectral and finite-volume approaches show consistent predicted behavior of the interplay between numerical and modeling errors for different model-discretization combinations. Of those studied here, the two most optimal combinations are identified as: (1) standard or dynamic Smagorinsky SGS model with a bounded central difference scheme; and (2) Monotonic Integrated LES (MILES) with either a second-order upwind or QUICK scheme. These combinations were applied for an axisymmetric jet flow at Re ∼ 10^5, using an ‘engineering quality’ mesh, where the MILES model with either an upwind or QUICK scheme showed the best predictive capability.

Keywords: turbulence modeling; large eddy simulation; eddy viscosity; discretization; finite-volume methods

1. Introduction

As available computing resources have continued to increase, large eddy simulation (LES) has grown in popularity among researchers and engineers for use in computational fluid dynamics (CFD) analysis of complex turbulent flows. The use of LES is motivated by a desire to compromise between the efficiency of Reynolds-averaged Navier-Stokes (RANS) and the theoretical accuracy of direct numerical simulation (DNS). While DNS for most high-Reynolds number engineering applications remains decades away, LES (or hybrid RANS/LES variants) are gradually becoming a common approach to problems with complex geometries and flow features in a number of application areas (Hanjalic, 2005). To date, most LES studies can be classified into one of two groups. The first is ‘fundamental’ studies, in which the subgrid stress (SGS) modeling aspects of LES are carefully studied using advanced simulation methods, such as spectral and pseudospectral techniques, for simple canonical flows. The second is ‘application’ studies, in which LES is used to solve problems of engineering relevance involving complex geometries and flow features, using readily available numerical methods and models. For example, Shalaby, Wozniak, & Wozniak (2008) performed LES for flow in a gas cyclone separator for industrial applications; Abdalla, Cook, & Hunt (2009) studied the dispersion characteristics of a buoyant plume above a point heat source using LES; and Su, Li, Li, Wei, & Zhao (2012) used LES to study complex vortical flow in a Francis turbine. In these cases, in order to validate the predictive capability of LES, results are usually analyzed by comparison with experimental data and/or other modeling methods (e.g., RANS). In many of these studies, the focus is on obtaining ‘good’ (i.e., engineering accurate) results using available general-purpose CFD tools. However, unlike their RANS counterparts, a detailed verification analysis is seldom performed to quantify numerical uncertainties and report on the accuracy of the solutions. One reason for the lack of such an analysis for LES is the strong coupling of SGS modeling and discretization errors, as both are functions of grid size.

Several authors have performed parametric studies to identify the best combination of modeling and numerical method, in terms of accuracy and computational cost. Baxevanou and Fidaros (2008) compared predictions using different combinations of k-ε and k-w RANS turbulence models and numerical schemes for transient...
flow over an ONERA-A airfoil. The study concluded that total variation diminishing (TVD) schemes show faster convergence and more accurate predictions than upwind and central-difference schemes for both turbulence models, and recommended them for engineering applications. Robertson, Choudhury, Walters, & Bhushan (2014) performed a parametric study to identify the most stable and accurate RANS and hybrid RANS/LES turbulence model and numerical scheme combination available in OpenFOAM. The study concluded that a second-order upwind scheme with limiters is the most stable, has the smallest computational cost, and provides the most accurate results for RANS simulations. Among the hybrid RANS/LES models, an improved delayed Detached Eddy Simulation (DES) model with a second-order bounded central difference scheme was identified to be the most accurate. The interplay of SGS modeling and dissipative discretization errors have been intentionally utilized for LES modeling by Boris, Grinstein, Oran, & Kolbe (1992), which are referred to as the monotonically-integrated LES (MILES) approach.

The objective of this paper is to evaluate different combinations of turbulence (SGS) models and numerical schemes for complex turbulent flows. For this purpose, modeling and discretization errors are assessed using both a pseudospectral solver and a commercially-available, general-purpose finite-volume solver (Ansys FLUENT® version 6.3), focusing on errors associated with the most commonly used second-order discretization schemes and Smagorinsky, dynamic Smagorinsky and MILES SGS models. Error assessment using pseudospectral techniques focuses on the evaluation of the effect of finite-differencing and modeling errors. For this purpose the pseudospectral code was modified to explicitly include the effects of finite-differencing errors for several different numerical schemes. This allows modeling and numerical errors to be isolated from one another, which is not possible in actual finite-volume CFD simulations. Error assessment using the finite-volume solver focuses on the identification of optimal combinations of SGS model and numerical discretization scheme for the best LES predictions using application solvers. Error analysis is performed for high-Reynolds-number decaying isotropic turbulence, matching an experimental test case available in the literature (Kang, Chester, & Meneveau, 2003), and previously validated LES predictions (Bhushan & Warsi, 2005). The optimal combinations of SGS model and numerical discretization scheme are then applied to the LES of a high-Reynolds-number Re ≈ 10^5, axisymmetric turbulent jet flow in order to validate their effectiveness.

2. Error analysis in LES

The governing equations for LES are obtained by filtering the Navier-Stokes equations, which for incompressible flow in divergence (conservative) form are

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}; \quad i,j \quad 1, 2, 3,
\]

where, \( \bar{u}_i \) is the filtered velocity field, \( \rho \) is the fluid density, \( \bar{p} \) is the filtered pressure field, \( \nu \) is the kinetic energy, and \( \tau_{ij} \) is the subgrid (or subfilter) stress tensor, and

\[
\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i u_j.
\]

The subgrid stresses must be modeled for closure of the governing equations. In practice, for LES with finite resolution, filtering may be either explicit or implicit and consists of two operations: convolution of the velocity field with the filter kernel, and projection of the continuous velocity field onto a discrete representation (Carati, Winkelmanns, & Jeanmart, 2001). We focus here on finite-volume numerical methods, in which the volume averaging procedure acts as an implicit filter, the net result of which is equivalent to convolution with a box filter kernel and the removal of all scales of motion beyond a cutoff wavenumber \( \kappa_c = \pi / \Delta \), where \( \Delta \) is the grid spacing. The box filter is smooth in spectral space, so that there is a subfilter component associated with all scales of motion, including the subgrid scales with a wavenumber less than \( \kappa_c \). It has been pointed out that the use of smooth filtering results in some ambiguity regarding the strict definition of the subgrid stresses (De Stefano & Vasilyev, 2002). Herein, we adopt the point of view that the subgrid stresses represent the net effect of all unresolved motion on the resolved flow field. The modeling error may then be defined for any realization of the resolved flow field as the difference between the modeled SGS tensor and the exact SGS tensor, as shown in Figure 1.

![Figure 1](image-url)

Figure 1. Implicit filtering due to volume averaging, indicating resolved and modeled (SGS) portions of the energy spectrum. The cutoff wavenumber \( \kappa_c \) is dictated by the grid size.

(Pope, 2000, Eq. 2.94):

\[
\frac{\partial \bar{u}_i}{\partial t} = 0, \quad (1)
\]

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}; \quad i,j \quad 1, 2, 3,
\]
In addition, LES suffers from numerical error due to the discretization scheme used to approximate Eqs. (1) and (2). A formal analysis of discretization errors was presented by Ghosal (1996), in which two contributions were identified: aliasing error due to discrete computation of the nonlinear term in Eq. (2), and finite-differencing error due to the inability of the numerical differentiation operators to represent derivatives exactly, especially at high wavenumbers. The former is well understood for pseudospectral methods and can be minimized using dealiasing techniques (Canuto, Hussaini, Quarteroni, & Zang, 1988; Collis, 2001). In finite-volume LES with second-order discretization schemes, aliasing error is usually associated with the assumption that variable values are uniform over each face of a computational control volume. Finite-differencing errors are associated with the accuracy of the specific discretization scheme, and are principally due to the differentiation of the nonlinear terms (Chow & Moin, 2003; Kravchenko & Moin, 1997). Several studies have found that for LES with sharp cutoff filters, both aliasing and finite-differencing errors are generally larger than the total effect of the SGS model, especially in the high-wavenumber portion of the flowfield (Chow & Moin, 2003; Fedioun, Lardjane, & Gokalp, 2001; Ghosal, 1996). In general, numerical errors are dominated by finite-differencing errors for lower-order schemes and aliasing errors for higher-order schemes.

Park, Yoo, and Choi (2004) found that there exists an optimum degree of upwinding for a scheme of a given order in which the sum of the finite-differencing and aliasing errors is minimized. They also demonstrated that spectral analyses of static error contributions were misleading, and that a dynamic analysis was necessary to accurately assess the combined influence of errors on real LES simulations. Fedioun et al. (2001) pointed out that analysis of aliasing and finite-differencing errors obtained using pseudospectral simulations with modified wavenumbers is in fact not equivalent to the results obtained with actual finite-volume simulations. This is due to the fact that representations in the physical and spectral space do not transform exactly. They developed a modified approach to error analysis using pseudospectral simulation and showed that the two numerical error sources coupled with the modeling error combined to yield good results for the case of a second-order central difference scheme and a fourth-order compact scheme (Kravchenko & Moin, 1997). Their simulations were performed using both convective and divergence forms for the nonlinear term:

\[
\frac{\partial \langle \bar{u}_i \bar{u}_j \rangle}{\partial x_j} : \text{divergence form; } \quad (4a)
\]

\[
\bar{u}_i \frac{\partial \bar{u}_j}{\partial x_j} : \text{convective form. } \quad (4b)
\]

It was demonstrated that the convective form yielded superior results. We note here that finite-volume codes almost exclusively adopt the divergence form for the nonlinear term in order to satisfy the conservation properties of the numerical scheme. It must also be noted that the results in Fedioun et al. (2001) were obtained using spectral eddy viscosity to model the SGS stresses, following the concept introduced by Kraichnan (1976). Such a model is difficult to implement into finite-volume simulations in physical space, which tend to rely on Smagorinsky-type eddy-viscosity models and are therefore likely to introduce greater amounts of modeling error, particularly in the higher wavenumbers.

This paper extends the previous analyses of modeling and discretization errors in LES to general-purpose finite-volume solvers using readily available numerical schemes and SGS models. The analysis proceeds in two parts. First, a pseudospectral code is used to evaluate the combined influence of SGS model and numerical flux formulation on the dynamical behavior of the LES of decaying isotropic turbulence. For this purpose, the numerical flux formulations use three different finite-differencing schemes: second-order central, second-order upwind (Barth & Jespersen, 1989), and the QUICK scheme (Leonard, 1979). Such relatively low-order formulations are used since these are most commonly employed in general-purpose CFD solvers. The evaluated SGS models include Smagorinsky (SM; Smagorinsky, 1963), dynamic Smagorinsky (DSM; Lilly, 1992) and no-model (denoted NM or MILES). The unmodified pseudospectral results obtained for each SGS model represent reference LES cases. In the second part of the paper, results are obtained for the same cases as above in physical space using the general-purpose finite-volume code Ansys FLUENT®. The results are assessed in terms of the relative strength of the SGS and numerical error contribution to dissipation, and the predicted energy spectra. Finally, suitable combinations of SGS model and numerical discretization scheme are determined, and several combinations are tested for the LES of a high-Reynolds-number, momentum-conserving, axisymmetric turbulent jet.

It must be noted that in LES simulations, the grid size (or filter size) dictates the level of resolved turbulence prediction. Thus for DNS grid resolutions, LES is expected to resolve the entire turbulence scale similar to DNS. The dependence of SGS model on grid size \( \Delta \) in Eq. (7) ensures that the effect of SGS model (and associated modeling error) decreases asymptotically with grid refinement. Numerical errors show a similar dependence on grid resolution and are expected to asymptotically decrease with grid refinement. Therefore, net error in a LES calculation for a given grid size is due to coupled SGS modeling and discretization errors.

3. Isotropic decaying turbulence test case

The first test case considered here is high-Reynolds-number decaying isotropic turbulence experimentally
investigated by Kang et al. (2003). The experiments were performed for spatially decaying turbulence for up to $\text{Re}_{\lambda} = 720$, where $\lambda$ is the Taylor length scale, using an inlet turbulence generator of size $M = 0.152$ m. In the experiment, the turbulent energy spectra were measured at downstream locations $x/M = 20, 30, 40$ and 48. The average streamwise velocity was $u_1(x) = 12.0, 11.2, 11.0$ and 10.8 m/s at $x/M = 20, 30, 40$ and 48, respectively. As summarized in Table 1, the turbulent characteristics at $x/M = 20$ included: turbulence intensity $u_1, \text{rms} = 1.85$ m/s; $\text{Re}_{\lambda} = 3.06 \times 10^4$, where $\ell$ is the integral length scale; $\ell/\eta = 2272$, where $\eta$ is the dissipation length scale; and $\ell/\lambda = 43$, where $\lambda$ is the Taylor microscale. The turbulence decays downstream and the characteristics at $x/M = 48$ included: $\ell/\eta = 1844$ and $\ell/\lambda = 37.8$.

### 3.1. Numerical simulation setup

Temporal LES computations were performed in a periodic cubic box. The box size was selected to be $2\pi$ m per side for the pseudospectral simulations, and 2.56 m per side for the finite-volume simulations. Numerical simulations were initialized using the experimental energy spectrum at $x/M = 20$ and results compared against experimental data at $x/M = 30, 40$ and 48. The flow parameters were scaled from the experiment to the numerical simulation, using the length scale ratio

$$l^* = \frac{L_{\text{Exp}}}{2\pi} = 0.81487, \quad (5a)$$

where, $L_{\text{Exp}} = 5.12$ m is the length of the decaying turbulence region reported in the experiment. The velocity scale is based on the turbulence intensity $u_1, \text{rms}$. The reference velocity in the simulation is chosen to be 2 m/s, which is the upper bound of the turbulence intensity in the experiment. The velocity ratio is:

$$u^* = \frac{u_{1,\text{rms}}}{2 m/s} = 0.9285. \quad (5b)$$

The Reynolds number of the flow is computed based on the turbulence intensity and grid size of the turbulence generator:

$$\text{Re} = \frac{1}{u^* l^*} \frac{u_{1,\text{rms}} M}{\nu} = 2.47 \times 10^4. \quad (5c)$$

The measurement locations downstream of $x/M = 20$ were converted into simulation times by using Taylor’s hypothesis:

$$t = \frac{x}{\int_0^x u_1(x)} \quad (5d)$$

Thus, $x/M = 30, 40$ and 48 correspond to $T = 0.1491, 0.3049$ and 0.4318 seconds, respectively.

The initial velocity field for the pseudospectral simulations was specified using random phases following Rogallo

| Case | Experiment (Kang et al. 2003) | LES studies in literature | Present study |
|------|-----------------------------|---------------------------|--------------|
| $L$  | $2\pi$ m; $N^3 = 128^3$; $h = 40$ mm | Pseudospectral: $L = 2\pi$ m; $N^3 = 64^3$; $h = 98$ mm | $L = 2.56$ m; $N^3 = 64^3$; $h = 40$ mm |
| $L$  | $L = 2\pi$ m; $N^3 = 64^3$; $h = 40$ mm | Margolin et al. (2006) | Bhushan et al. (2006) |

Table 1. Summary of turbulent characteristics and grid resolution used in LES studies available in the literature and in the present study.
(1981), with an energy spectrum reported by experiments (Kang et al., 2003) with Eq. (5e):

\[
E(\kappa) = C_K \kappa^{2/3} \kappa^{-5/3} \left( \frac{\kappa \ell}{\sqrt{\varepsilon}} \right)^{\frac{3}{2}} e^{-\alpha_1 \kappa \eta} \times F(\kappa \eta),
\]

(5e)

where, \(\epsilon\), \(\ell\), and \(\eta\) are the experimentally reported values at the \(x/M = 20\) measurement plane. The constants \(C_K\) and \(\alpha_1 - \alpha_2\) are 1.613, 0.39, 1.2, 4.0 and 2.1, respectively. The factor \(F\) represents the bottleneck effect on the energy spectrum, but the simulations in the present work used a sufficiently large filter width such that accurate spectra were represented with \(F = 1\). The initial flow field was run for a sufficient length of time until the skewness achieved a steady state and the initial random phases adjusted to a physically representative turbulent state. The velocity field was then rescaled in Fourier space to match the energy spectrum at \(x/M = 20\), and the simulation was performed using the adjusted flow field (Kang et al., 2003; Walters & Bhushan, 2005).

For the finite-volume simulations using Ansys FLUENT®, the initial energy spectrum in Eq. (5e) was modified using the spectral box filter function \(G(\kappa)\) to include the effect of the box-filtering operator implicit in the finite-volume formulation

\[
E_{box}(\kappa) = G^2(\kappa)E(\kappa) = \frac{\sin(\kappa \Delta)}{\kappa \Delta}^2 E(\kappa).
\]

(6)

The velocity field was specified using 30 discrete wavenumbers spanning length scales ranging from the Kolmogorov scale \(\eta\) to 10\(\ell\). The wavenumbers were logarithmically equispaced with a ratio of 1.122. The velocity field was specified with 16 modes per wavenumber.

Pseudospectral simulations were performed using 32\(^3\) and 64\(^3\) grid resolutions. The averaged grid resolution characteristics for the 32\(^3\) case are: \(\ell/h = 1.5\), \(h/\lambda = 26\) and \(h/\eta = 1306\). The grid characteristics of the 64\(^3\) case are: \(\ell/h = 3\), \(h/\lambda = 13\) and \(h/\eta = 653\), as summarized in Table 1. Both the grids have resolution \(h/\eta < \ell/\eta\) — however, for the coarse grid, the grid resolution is barely fine enough to resolve the largest energy-containing length scales. Therefore, this study focuses mostly on the finer 64\(^3\) grid. This grid is sufficiently fine such that the grid scale is located in the inertial subrange. Thus it is expected that the simulations will resolve the largest energy-containing eddies. However, considering large \(h/\lambda\) values, the grid is not fine enough to resolve all of the inertial subrange turbulent structures. Since the objective of the study is to investigate the best practices for practical LES applications for engineering problems, a grid resolution fine enough to resolve fine-scale turbulence is not warranted. Note that the 64\(^3\) grid resolution has been successfully used by other pseudospectral studies for this particular test case with a variety of subgrid closures. For example, Hickel, Adams, and Domaradzki (2006) used the same grid for the validation of an adaptive local deconvolution method for LES. Margolin, Rider, and Grinstein (2006) used this grid for the validation of the implicit LES methodology, and reported that their results on the 64\(^3\) grid are consistent with the 128\(^3\) results reported in the literature. Bhushan, Warsi, and Walters (2006) used the grid for the validation of an algebraic model for LES. The study also included LES simulation using a dynamic Smagorinsky model.

Finite-volume simulations were performed using a 64\(^3\) grid for which averaged \(\ell/h = 7.45\), \(h/\lambda = 5.4\) and \(h/\eta = 267\). The grid resolution is same as that used by Kang et al. (2003) for their LES study. Note that we have considered a finer grid for finite-volume simulations compared to pseudospectral simulations, as the former is expected to have higher numerical error than the latter.

The time step for the simulation was \(\Delta t = 0.00074\) and 0.00037 for the 32\(^3\) and 64\(^3\) grid cases, respectively. The time step size is an order of magnitude smaller than the time scale of the resolved turbulence eddies. It is expected that time discretization will have negligible impact on results.

The subgrid stresses were modeled as:

\[
\tau_{ij} = -2C_S \Delta^2 \sqrt{2S_{ij}} S_j, \quad (7)
\]

where, \(C_S\) is a model coefficient, \(\Delta\) is the grid size, and \(S_j = \frac{1}{2} \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right]\) is the rate-of-strain tensor. The study uses both SM and DSM models. For SM, \(C_S = 0.03\) and 0.01 for isotropic decaying turbulence and free-shear jet flows, respectively (Bhushan & Warsi, 2007; Pope, 2000). For DSM, \(C_S \Delta^2\) is computed dynamically at every time step for the domain, using explicit filtering and using the scale-similarity assumption (Lilly, 1992). Simulations were also performed without any turbulence modeling, i.e., \(\tau_{ij} = 0\). For the pseudospectral simulations, these simulations are referred to as no-model (NM). The finite-volume simulations include dissipative finite-differencing errors, therefore such cases correspond to MILES (Boris et al., 1992), wherein the numerical dissipation replaces subgrid dissipation.

### 3.2. Calculation of energy spectra

To compute the energy spectra from the LES results, a fast Fourier transform (FFT) was performed for the velocity field (not required for the pseudospectral code) to obtain the Fourier components of the velocity \(\hat{u}_j\) in 3D wavenumber space, \(\kappa_j = [-N/2 \ldots 0 \ldots N/2 - 1]\), where \(j = 1,2,3\) correspond to the three spatial dimensions, and \(N\) is the number of grid points in each direction of the domain. The data is then organized in the wavenumber space, such that wavenumbers \(\kappa_1 = 0\), \(\kappa_2 = 0\) and \(\kappa_3 = 0\) lie at the center. A spherical domain is defined with the radius \(\kappa = \sqrt{\kappa_1^2 + \kappa_2^2 + \kappa_3^2}\) = \([0, N/2 - 1]\) and the velocity field is interpolated.
onto the surface of the domain. Note that repeated subscript notation represents summation. The energy spectrum is then obtained by numerical integration on the surface of the domain \( ds \) as below:

\[
E(\kappa) = \frac{1}{4\pi \kappa^2} \int \int \hat{u}_j \hat{u}_j^* ds,
\]

where \( * \) denotes the conjugate component of the complex variable.

4. Pseudospectral simulation methodology

4.1. General methodology

The Fourier-Galerkin approximations of Eqs. (1) and (2) are (Bhushan & Warsi, 2007):

\[
\begin{align*}
\frac{d}{dt} + v \kappa^2 \hat{u}_i(\kappa) &= 0, \quad (9a) \\
\left( \frac{d}{dt} + v \kappa^2 \right) \hat{u}_i(\kappa) &= -ik_j \frac{1}{\rho} \hat{p}(\kappa) - \hat{u}_j \hat{u}_j(\kappa) + \hat{\tau}_{ij}(\kappa), \quad (9b)
\end{align*}
\]

where \( \hat{u}_i \) and \( \hat{p} \) represent the Fourier coefficients of the velocity and pressure as functions of the discrete wavenumber vector \( \kappa \). The second term on the right in Eq. (9b),

\[
- \hat{u}_j \hat{u}_j(\kappa) = \hat{\tau}_{ij}(\kappa) = \hat{f}_i(\kappa),
\]

is the spectral representation of the nonlinear convection term. The pressure term in Eq. (7) can be eliminated by substituting Eq. (8) (the continuity equation) into Eq. (9) as

\[
\hat{p}(\kappa) = -ik_j \hat{f}_j(\kappa)/\kappa^2.
\]

The resulting ordinary differential equation that is integrated in time in the pseudospectral simulations is therefore

\[
\frac{d}{dt} \hat{u}_i(\kappa) = \hat{f}_i(\kappa) - \kappa_k \kappa_j \hat{f}_j(\kappa)/\kappa^2 - v \kappa^2 \hat{u}_i(\kappa).
\]

The local time derivative is advanced by a second-order Runge-Kutta scheme. The nonlinear term and the SGS term on the right-hand side are determined by using the inverse FFT to compute the velocity field, evaluating the terms in physical space, and taking the FFT to yield their spectral representation. Since the governing equations are solved in wavenumber space, the solver involves (implicit) sharp spectral filtering. A 3/2-rule was employed to minimize aliasing errors (Collis, 2001), such that finite-difference errors could be isolated and studied.

4.2. Approximation of finite-differencing errors

Approximation of finite-differencing errors is accomplished by adding an error term to the spectral representation of the Navier-Stokes equations. In order to avoid any difficulties associated with the spectral representation of finite-difference errors, an alternative to the modified wavenumber method is employed, in which the error terms are evaluated using a Taylor series expansion in physical space and their spectral contribution is computed using the FFT.

The numerical errors that are investigated are those due to the numerical approximation of the derivative appearing in the convection term, which are expected to be the dominant contributing factor to the total numerical error (Fedoum et al., 2001). Defining the operator \( \frac{\partial}{\partial x_j} \) as the difference between the numerical (denoted by \( \text{DISC} \)) and exact derivative (denoted by \( \text{EXACT} \)),

\[
\frac{\delta}{\delta x_j} = \frac{\partial}{\partial x_j} \text{DISC} - \frac{\partial}{\partial x_j} \text{EXACT},
\]

the numerical error in the convective term is

\[
e_i = \hat{u}_j \frac{\delta u_i}{\delta x_j}.
\]

The differentiation error operator in Eq. (13) can be constructed from the truncated terms in the Taylor series expansion of the different finite-differencing schemes, which results in:

Central differencing (CD):

\[
e_i = \hat{u}_j \left\{ \frac{\Delta^2}{6} \frac{\partial^3 \hat{u}_i}{\partial x_j^3} + \frac{\Delta^4}{120} \frac{\partial^5 \hat{u}_i}{\partial x_j^5} + \frac{\Delta^6}{5040} \frac{\partial^7 \hat{u}_i}{\partial x_j^7} + \ldots \right\}
\]

Second-order upwind (2U):

\[
e_i = -\hat{u}_j \left\{ \frac{\Delta^2}{3} \frac{\partial^3 \hat{u}_i}{\partial x_j^3} + \frac{\Delta^3}{4} \frac{\partial^4 \hat{u}_i}{\partial x_j^4} + \frac{7 \Delta^4}{60} \frac{\partial^5 \hat{u}_i}{\partial x_j^5} + \ldots \right\}
\]

QUICK (Q):

\[
e_i = -\hat{u}_j \left\{ \frac{13 \Delta^2}{48} \frac{\partial^3 \hat{u}_i}{\partial x_j^3} + \frac{7 \Delta^3}{32} \frac{\partial^4 \hat{u}_i}{\partial x_j^4} + \frac{97 \Delta^4}{760} \frac{\partial^5 \hat{u}_i}{\partial x_j^5} + \ldots \right\}
\]

It must be noted that in order to preserve the upwinding nature of the two 2U and Q schemes, the errors involving even derivative terms are multiplied by the absolute value of the velocity, \( |\hat{u}_j| \), as derived in Appendix 1. An exact representation of the error would require the retention of all of the truncated terms, which is both impossible and unnecessary. As discussed later, numerical experiments were performed to determine the minimum number of terms that need to be retained in order to accurately approximate the numerical error.

The numerical errors computed using Eqs. (14) are added in Eq. (12) to obtain the modified LES equations:

\[
\frac{d}{dt} \hat{u}_i(\kappa) = \hat{f}_i(\kappa) - \kappa_k \kappa_j \left( \hat{f}_j(\kappa) + \hat{c}_j(\kappa) \right)/\kappa^2 - v \kappa^2 \hat{u}_i(\kappa) + \hat{c}_i(\kappa),
\]

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where \( \hat{e}_i(\kappa) \) is the spectral representation of the numerical error in physical space given by \( e_i(x) \). It must be noted that the calculation of higher-order derivative terms is simple in the pseudospectral solver, as it reduces to a simple arithmetic operation, i.e., FFT of \( \left[ \frac{\partial^2 u}{\partial x^2} \right] = (i\kappa)^2 \hat{u} \).

5. Finite-volume simulation methodology

Finite-volume simulations were performed with the commercial flow solver Ansys FLUENT®. The solution algorithm was fully implicit and the time-dependent term was discretized using a second-order backward difference approximation. The simulations used the segregated solver, with which continuity and momentum equations were solved in a decoupled fashion during the outer iteration loop. The time advancement was carried out using non-iterative time advancement (NITA), i.e., a single outer iteration was performed during each time step, and the fractional step method was used for pressure-velocity coupling (Glaz, Bell, & Colella, 1993). The dimensionless time step size was the same as in the pseudospectral simulations. The efficacy of the NITA scheme was evaluated by comparison with an iterative (implicit) time advancement scheme that incorporated the SIMPLE algorithm (Patankar & Spalding, 1972) for pressure-velocity coupling and 25 outer iterations per time step. The results using both methods were found to be identical, but the NITA scheme reduced the computational time by an order of magnitude versus the iterative SIMPLE scheme.

Second-order extrapolation was used to evaluate the pressure at the control volume faces, and convective fluxes were evaluated at each face using several different spatial discretization schemes. These included the second-order central difference (CD), upwind (2U), QUICK (Q) and bounded central difference (BCD) schemes. The first-order upwind scheme (1U) was also used for comparison purposes. The BCD scheme is an adaptive scheme that represents a mixture of second-order central and upwind differencing, and first-order upwind differencing when the convection boundedness criterion is violated. This scheme potentially approximates a near-optimum scheme defined by Park et al. (2004), which includes just the right amount of dissipation to minimize the sum of aliasing and finite-differencing errors. SM, DSM and MILES were used for SGS modeling.

6. Isotropic decaying turbulence results

6.1. Pseudospectral simulations

The first necessary step in the error analysis was to determine the appropriate number of terms that need to be retained in the Taylor series expansion of the numerical discretization in Eqs. (14). To do this, simulations were conducted using a successively larger number of terms to represent the numerical differentiation error, i.e., SM-3 retains only 3rd derivative term, SM-34 retains 3rd and 4th derivative terms and SM-345 retains up to 5th derivative term. Figure 2 shows that retention of terms up to fifth-order error for the 2U scheme in Eq. (14c) does not show significant change in the computed energy density spectrum compared to retention of up to fourth-order error terms. It is expected that retention of even higher order terms will not lead to significant changes. Similar results were obtained for the CD and Q schemes, for which retention of seventh- and fifth-order error terms, respectively, did not show significant changes in the energy density spectrum. As a result, Eq. (14b) was truncated after the seventh-order derivative term and Eqs. (14b) and (14d) were truncated after the fifth-order derivative term. The naming convention used in the remainder of this section is to state the SGS model label first, followed by the (approximated) numerical discretization scheme label second. The absence of a second label indicates the unmodified pseudospectral result. For example, SM denotes pure pseudospectral LES with the constant-coefficient Smagorinsky model, while DSM-CD implies pseudospectral LES with the dynamic Smagorinsky model and added error contribution from the CD numerical flux formulation.

Figure 3(a) shows results on the \( 32^3 \) grid using the Smagorinsky SGS model in conjunction with numerical error from all three numerical schemes. The results highlight the dissipative nature of the upwind biased schemes. This effect is most apparent at higher wavenumbers, where the results clearly indicate that there is an excessive removal of energy and underprediction of the experimental data. SM-CD shows a pile up of energy at high wavenumbers, as the dispersive error of the CD scheme dominates the dissipative influence of the SGS model. It is clear from Eq. (14b) that the error term for the CD scheme is symmetric and does not remove kinetic energy from the system. The \( 64^3 \) grid predictions in Figure 3(b) are similar to those of the \( 32^3 \) grid for all of the schemes. The
DSM model with upwind biased schemes, as shown in Figure 4(a), shows a trend similar to the SM model. It should be noted that the DSM-CD solution diverged due to excess dispersion and non-physical energy pile up at high wavenumbers, which clearly demonstrates the nonlinear interaction between SGS models and numerical schemes. The eddy-viscosity coefficient in the DSM is dependent on the resolved strain-rate rather than on a fixed coefficient, hence the dissipative influence of this model is not sufficient to stabilize the simulation against the effects of the CD scheme. The NM simulations in Figure 4(b) showed predictions similar to SM and DSM for the upwind scheme, and diverged for the CD scheme, similar to DSM predictions.

Figures 3 and 4 show that NM simulations predict lower energy content than the SM and DSM cases, suggesting that NM has higher dissipation than SM or DSM. This is in contrast to the expectation that turbulence models will result in additional dissipation over NM. It must be noted that the results shown in Figures 3 and 4 are only at an instant, and do not show the turbulent kinetic energy (TKE) decay predicted by different models. Analysis of the TKE decay pattern reveals that NM simulations show excessive decay of TKE early on in the simulations, and show lower decay than SM and DSM later on in the simulations. The early excessive decay results in a lower TKE profile overall than SM and DSM. The early excessive dissipation in NM is likely due to inaccurate development of small-scale turbulence structures. However, it is apparent that the discretization scheme plays a more significant role than the SGS model in determining the predicted energy spectrum, particularly in the high-wavenumber regions. This suggests that the choice of SGS model may be of minor importance in ‘application’ LES simulations using general-purpose solvers with common second-order schemes. It also suggests that conclusions regarding model performance obtained using high-fidelity (e.g., pseudospectral) solvers in ‘fundamental’ LES studies will not necessarily translate to practical LES, and that care must be taken to ensure that any SGS model is not simply adding extra dissipation in an ad hoc fashion. Finally, it should be noted that these results do not reflect the influence of solid boundaries in wall-bounded flows. In such a case, it is expected that the combination of grid and SGS model will in fact play a
critical role, but detailed investigation of such situations is beyond the scope of this work.

6.2. Finite-volume simulations

Results analogous to those above are presented in this section, obtained using the general-purpose finite-volume solver. Energy spectra corresponding to the downstream-most measurement station in the experiments are shown in Figures 5(a) and 5(b) for the SM and DSM simulations, respectively. As is evident, the BCD and CD scheme predictions are similar and show good agreement with experiments at the low wavenumbers. However, the former is underpredictive and the latter overpredictive at larger wavenumbers. Results with the 2U, Q, and 1U schemes show a substantial amount of dissipation, as expected. The 1U scheme is overly dissipative even at low wavenumbers, and the 2U and Q schemes provide similar energy spectra to each other. The energy spectrum obtained using MILES in Figure 5(c) shows the best agreement with experiments using either the BCD or Q schemes, although there is a slight overprediction of the energy in the lower wavenumbers with the Q scheme. The MILES-Q result is arguably as good as the DSM-BCD result in terms of the energy spectrum, although its formulation is much simpler both in terms of the numerical method and the SGS model. Interestingly, the MILES-BCD results show the best agreement with experiments over the entire energy spectrum. The MILES-CD result, not surprisingly, is highly dispersive and nonphysical. Overall, the finite-volume simulation results showed similar behavior to the pseudospectral simulations, including the dissipative nature of the upwind biased schemes and energy pile up in the high wavenumbers for the central difference scheme. In particular, the observation above, that numerical scheme plays a greater role in determining the predicted spectral behavior than the SGS model, is supported in the finite-volume results.

Results from the finite-volume simulations were analyzed to evaluate the net dissipative contribution from each of three sources — the discretization scheme, the SGS model, and the viscous stress terms. The total dissipation was estimated based on the time derivative of turbulent kinetic energy, \( \frac{dk}{dt} \), at each time step. The SGS and viscous dissipation were estimated based on their volume averages within the domain at each time step, i.e.:

\[
\text{SGS Dissipation: } \varepsilon_{\text{SGS}} = \oint \nu (2S_{ij}S_{ij})^2 dV; \tag{16a}
\]

\[
\text{Viscous Dissipation: } \varepsilon_{\text{visc}} = \oint \nu (2S_{ij}S_{ij})^2 dV. \tag{16b}
\]

The numerical dissipation was calculated as the difference between the total and the SGS + viscous dissipation:

\[
\text{Numerical Dissipation: } \varepsilon_{\text{Num}} = \frac{d}{dt} \oint k dV - \varepsilon_{\text{SGS}} - \varepsilon_{\text{visc}}. \tag{16c}
\]

Figure 5. Finite-volume simulation energy spectra obtained for isotropic decaying turbulence using (a) Smagorinsky model, (b) dynamic Smagorinsky model and (c) MILES with different numerical schemes, are compared with experimental data at \( x/M = 48 \).

The computed viscous dissipation was found to be negligible for this case, which is expected since the mesh size is much larger than the Kolmogorov length scale.

The relative contribution of the numerical error from four of the discretization schemes, for simulations using the Smagorinsky model, is shown in Figure 6. It is clear that the more dissipative the scheme, the higher the contribution of numerical dissipation. Similar results were found for the cases using DSM. For all of the MILES simulations, of course, almost 100% of the dissipation arises due to the
numerical scheme. What is most relevant from Figure 6 is the fact that two of the schemes, CD and BCD, have smaller contributions to the overall dissipation from the numerical scheme than from the SGS model. For the Q scheme, approximately 65% of the dissipation arises due to numerical error, and only about 35% from the SGS model. The 2U scheme shows dissipation characteristics similar to the Q scheme, and results in only a net 3.5% higher numerical dissipation than the Q scheme. For the 1U scheme, not surprisingly, almost all of the dissipation is due to the numerical error. The results again confirm that for upwind-biased second-order schemes, the numerical error dominates over the contribution of the SGS model. Even for a less dissipative scheme such as BCD, the numerical contribution is almost equal to the SGS model contribution.

The predictive capability of the different combinations of SGS models and numerical discretization schemes are evaluated by estimating error in the prediction of energy spectra at $T = 0.13, 0.27$ and $0.38$ (which corresponds to experimental data at $x/M = 30, 40$ and $48$, respectively) using experimental data, and summarized in Table 2. For both SM and DSM models, the CD scheme shows the smallest error, due to overprediction of the energy spectrum at higher wavenumbers and underprediction for lower wavenumbers. BCD shows a 3% larger error than CD, whereas the 2U and Q schemes show up to 10% larger errors than the CD scheme. The 1U scheme again shows a significantly larger error of 49%. MILES using BCD provides the best prediction among the model-scheme combinations, for which the error is 2.73%. MILES using CD predicts errors of 34%, whereas errors predicted using the 2U and Q models are nominally less than 10%.

Overall, the analysis indicates that the use of an upwind-biased discretization scheme (either 2U or Q) enables reasonably accurate resolution of low wavenumber velocity modes, but high wavenumber modes cannot be resolved due to high levels of numerical dissipation. This result is of course not surprising. The central-difference scheme shows non-physical behavior in the energy spectrum and significant overprediction of the decay rate regardless of the SGS model. The BCD model shows the most accurate spectral resolution for all of the models.

Often, for engineering-level simulations, accurate resolution of high wavenumber velocity components is less critical than the accurate prediction of mean flow and large-eddy characteristics. Exceptions, for example acoustics simulations, generally require high-order/low-dissipation numerical schemes for accurate results. For more general flow analyses, these results indicate that the use of a second-order upwind scheme may in fact provide ‘engineering accurate’ solutions. Interestingly, for the decaying turbulence test case, the upwind-biased schemes apparently provide enough dissipation such that the addition of an SGS model is redundant, and may even decrease accuracy. This point underscores a more general observation, namely that conclusions drawn from fundamental LES studies regarding SGS model performance are often based on high-resolution (e.g., pseudospectral) numerical methods. Care must be taken when translating model performance characteristics to simulations using lower-resolution numerical methods, to ensure that SGS models are not merely adding extra dissipation to an already sufficiently dissipative solution.

### 7. Engineering application: round jet flow

To evaluate the above observations using a test problem more indicative of realistic engineering applications, simulations were performed using Ansys FLUENT® for a turbulent round jet flow issuing into a quiescent fluid. Three model-scheme combinations were selected for comparison, based on the results from the isotropic decaying turbulence simulations. These included two with the BCD scheme, which represents an advanced numerical method developed specifically for high-resolution simulations. The BCD scheme was combined with the DSM model – considered the most advanced of the eddy-viscosity SGS models investigated in this study – as well as with the SM model, which is a simpler and older model form but which showed better prediction of turbulence decay when paired with the BCD scheme. The third combination was
MILES-2U, which showed the best results in terms of the low wavenumber portion of the turbulence spectrum, and was found to be more stable than the MILES-BCD combination.

7.1. Test case
Simulations were performed to match the axisymmetric jet experiment of Hussein, Capp, & George (1994). The case included a relatively high Reynolds number (Re \( \approx 10^5 \)), and a Mach number equal to approximately 0.2. The experiment was performed in a facility large enough to be considered an infinite environment, and recirculation flow entrainment was avoided. The data were collected using laser doppler anemometer (LDA), single hot wire (SHW), and flying hot wire (FHW) techniques, and included: (1) mean centerline velocity at several downstream locations; (2) profiles of the mean streamwise velocity, and streamwise, radial and azimuthal turbulence intensities versus non-dimensional radial distance \( \eta = \frac{r - x_0}{x_0} \), where \( x_0 \) is the jet origin, from the jet centerline at 50D, 70D and 90D downstream of the jet; and (3) estimate of energy balance, and pressure-velocity and pressure-strain rate correlations. Herein, the centerline velocity and turbulence intensity data are compared to simulation results for validation purposes.

7.2. Simulation setup
Initial tests were performed to obtain an economical grid for the simulations, which involved evaluation of the appropriate outer domain location such that the boundary

Figure 7. (a) 2D schematic of the round jet domain, boundary conditions and grid at the jet exit for simulation setup (following Hussein et al., 1994). The domain dimensions are shown with respect to the exit Diameter \( D = 1 \) inch; (b) view of the O-type grid used along the azimuthal direction.
condition does not affect the flow (Adedoyin, 2007). For this purpose, a cylindrical domain of radius 60D and a smaller conical domain as shown in Figure 7(a) were considered. Simulations were performed on these domains using a coarse 1M grid, which showed no significant effect of outer domain on the results. Thus, in order to minimize the numerical expense, the smaller conical domain — as shown in Figure 7(a) — was used for the study. Since the objective of this study is to evaluate the interplay of modeling-scheme errors for engineering applications, and not to obtain the best results for the jet flow, a reasonably fine grid resolution — comparable to that used in engineering applications — was sought. Therefore, the grid was refined to obtain a grid consisting of approximately 3M cells. The grid design for the domain is shown in Figure 7(b).

The simulation domain in Figure 7(a) was built with an initial (upstream) diameter 5 times larger than the jet

![Diagram](image)

Figure 8. (a) Instantaneous streamwise velocity distribution in the jet. The inset figure shows the convergence history of the streamwise velocity component for SM-BCD; (b) Comparison of centerline velocity variation with distance from the jet exit for experimental data (Hussein et al., 1994) and MILES-2U, DSM-BCD and SM-BCD LES.
exit diameter ($D = 1$ inch), and the outer domain diameter grew at a rate of 0.5 inches per inch in the streamwise direction. The maximum streamwise domain extent was $115D$ downstream of the jet exit with a maximum outer diameter of $60D$. All of the outer boundaries external to the jet were specified as having a constant (ambient) pressure. This choice of boundary condition allows the low velocity entrainment of ambient fluid into the jet and accurately reproduces the effects of an infinite domain. The experimental study reported that the jet exit velocity closely resembled a top-hat profile with a laminar boundary layer thickness of $\delta_{95} = 0.7$ mm at the jet exit. To achieve the required boundary layer thickness at the jet exit, an inlet supply pipe was added for the simulation as shown. The length of the supply pipe ($x$) was estimated from the flat plate laminar boundary layer equation:

$$\frac{\delta}{x} = \frac{5}{Re^{0.5}}.$$  (17)

For jet exit velocity $U = 56.2$ m/s, this yields an inlet length of 3 inches. This supply tube length was used in the simulation, and a uniform velocity was applied at the supply tube inlet. Results showed that the predicted exit velocity profile closely matched the experimental profile. The time step size for the simulations was specified to have a maximum (convective) Courant–Friedrichs–Lewy (CFL) number of 1.0, which corresponded to $\Delta t \approx 10^{-6}$ s.

### 7.3. Results

Figure 8(a) shows a representative plot of the convergence history of the solution and the instantaneous contours of the streamwise velocity distribution in the jet at a statistically stationary state for the SM-BCD combination. Temporal convergence was assessed using the running time average of the streamwise velocity at a location $100D$ downstream of the jet exit. It took approximately 40 K time steps to achieve convergence for SM-BCD and MILES-2U, and 50 K time steps for DSM-BCD.

![Figure 9](image)

Figure 9. Comparison of mean velocity profile obtained using MILES-2U, DSM-BCD and SM-BCD LES with experimental data (Hussein et al., 1994) at downstream distance (a) 50D, (b) 70D and (c) 90D.
The instantaneous streamwise velocity contours in Figure 8(a) highlight the fundamental aspect of LES, namely that the large turbulent flow structures are well resolved in the simulation. Also apparent is the low speed entrainment of ambient fluid into the jet. Figure 8(b) compares the inverse of the centerline mean streamwise velocity versus the downstream distance with the experimental data. The virtual origin \( x_0 \) for the simulations was determined to be \( 4.9D \pm 0.6D \), upstream of the jet exit. All of the simulations show a linear increase, similar to what was observed in the experiment. In terms of centerline velocity decay, the MILES-2U slope predictions compare within 8% of the experimental data, while the SM-BCD and DSM-BCD slopes were underpredicted, indicating that turbulent mixing of mean momentum using both BCD combinations was less than that observed in the experiments. This suggests a complex interaction between numerical and model dissipation, and energy transfer mechanisms from large resolved to small resolved turbulent scales.

Consistent with the isotropic turbulence results above, the use of a more dissipative (upwind-biased) discretization scheme with no SGS model yields more accurate results than a less dissipative scheme with common eddy-viscosity SGS models.

In Figure 9, the radial profile of the normalized mean streamwise velocity is compared with the experimental data at the three downstream locations, for each of the three tested model-scheme combinations. The predicted profiles demonstrate self-similar behavior downstream, which is expected for the mean quantities. SM-BCD performs slightly better than the other models — however, the averaged error is reasonable (< 6%) for all the combinations.

Figures 10–12 compare the resolved turbulence intensity components with the experimental data at each downstream location. The turbulence intensity components show self-similar behavior, similar to the mean velocity profile. All combinations underpredict the turbulence intensity.
intensities close to the jet center, i.e., $0 \leq \eta \leq 0.06$, by up to 25–30%. An underprediction of the resolved turbulence intensity is expected in LES because the simulation does not resolve the entire turbulence scale, as in the experiment. LES comparison with experimental data can be improved by adding modeled turbulence intensity, which is unfortunately not available in the solutions, i.e., modeled turbulent kinetic energy is not computed in the SM, DSM and MILES simulations. Among the combinations considered, MILES-2U shows the highest resolved turbulence level, whereas no significant differences are observed between the SM and DSM predictions.

Overall, the results for the jet flow case show reasonable agreement with experiments, including self-similarity, good agreement for radial profiles of mean velocity, and reasonable agreement of radial profiles of second moments. The differences between the different model-scheme combinations manifest primarily in the prediction of centerline mean velocity. Surprisingly, but consistent with the results for decaying isotropic turbulence, the best agreement was found for the case of no-model (MILES) in combination with a second-order upwind discretization scheme.

8. Summary and conclusions
The goal of this research effort was to evaluate combinations of SGS model and discretization schemes for the LES of complex turbulent flows using general-purpose CFD algorithms, represented here by the commercial code Ansys FLUENT®. To achieve this goal, a formal quantification of coupled modeling and discretization errors present in finite-volume/finite-difference simulations was first conducted for isotropic decaying turbulence. The study focused on commonly used second-order finite-differencing schemes, as well as the Smagorinsky and dynamic Smagorinsky SGS models, and MILES (i.e., no SGS model). The errors were assessed using a pseudospectral solver, in which finite-differencing errors were added as explicit terms on the right-hand side of the spectral equation.

Figure 11. Comparison of radial turbulence intensity obtained using MILES-2U, DSM-BCD and SM-BCD LES with experimental data (Hussein et al., 1994) at downstream distance (a) 50D, (b) 70D and (c) 90D.
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representation of the governing momentum equations. This allowed the isolation of the two error sources due to modeling and numerical scheme. Following this, net modeling and discretization errors in the application solver were studied, and the optimal combinations of SGS model and numerical discretization scheme for the best LES predictions were identified. The effectiveness of the optimal combinations of model/scheme identified from the isotropic decaying case were applied for the LES of a high $Re \approx 10^5$ axisymmetric turbulent jet flow.

The interplay of the modeling and discretization errors shows a consistent behavior in both the pseudospectral and finite-volume simulations of isotropic decaying turbulence. Conclusions are summarized as:

1. the upwind and QUICK schemes are dissipative and appear to provide an appropriate level of dissipation when combined with the MILES approach;
2. the central-difference scheme shows dispersion errors, which helps in counteracting SGS errors in selected cases, but is not reliable as it leads to energy pile-up at higher wavenumbers;
3. the bounded central-difference scheme, which combines the effects of a central differencing scheme and an upwind scheme, helps to eliminate the energy pile-up issue of the central-difference scheme, and is found to be appropriate for SM and DSM simulations; and
4. MILES with second-order upwind or QUICK schemes performed better than MILES with BCD for the prediction of large-scale turbulent structures, and provided the best results for the engineering applications.

Taken in their entirety, the results from this study suggest that useful predictions may indeed be obtained from LES of engineering flows using commonly available discretization schemes and SGS models found in general-purpose flow solvers. Important guiding principles are that the discretization scheme should be non-dispersive, and

![Figure 12](image_url) Comparison of azimuthal turbulence intensity obtained using MILES-2U, DSM-BCD and SM-BCD LES with experimental data (Hussein et al., 1994) at downstream distance (a) $50D$, (b) $70D$ and (c) $90D$. 
that the combined effects of the discretization scheme and SGS model should provide a sufficient but not overly large level of dissipation. Satisfying these criteria has been found to result in a good prediction of the large-scale flow behavior, including the energy spectrum (except near the cutoff wavenumber), turbulent energy decay, and turbulent mixing dynamics. The four combinations investigated here that most closely meet this requirement are SM or DSM with bounded central-difference, and MILES with the second-order upwind or QUICK scheme. Perhaps surprisingly, it is the latter two, which rely on no explicit SGS model and on strongly upwind discretization schemes, that yield the best results overall for the test cases considered here.

More generally, the results suggest that the choice of SGS model may be of minor importance in ‘application’ LES simulations using general-purpose solvers with common second-order schemes, and that upwind-biased schemes apparently provide enough dissipation such that the addition of an SGS model is redundant, and may even decrease accuracy. It must again be pointed out that these conclusions are only applicable to the non-wall-bounded turbulent flows considered here, and it is expected that grid anisotropy and SGS model details will play a critical role in near-wall turbulence simulations. Although such an analysis is beyond the scope of this study, it should be considered as a future research effort.

Ongoing and future work efforts are focusing on the identification of the best model-discretization combination for hybrid RANS/LES models, since such models are gaining popularity in the CFD application community due to having lower grid resolution requirements than LES. Some initial results have shown that the choice of MILES for the LES mode with the BCD scheme shows improved resolved turbulence level predictions in comparison to the eddy viscosity type LES model (Walters, Bhushan, Alam, & Thompson, 2013). Future work will focus on a systematic study, similar to the present study, for hybrid RANS/LES models.

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**Note**

1. The no-model simulations are only designated as MILES for the finite-volume simulations, since the unmodified pseudospectral simulations do not include any dissipative numerical operators in their formulation, which are integral to the MILES approach.

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**Appendix 1. Numerical error for second-order upwind scheme**

For a 1D system, the error in the convection term is:

\[ e = \frac{\delta u}{\delta x} = \begin{cases} \frac{u_{BD}}{\delta x} : u \geq 0 \\ \frac{u_{FD}}{\delta x} : u < 0 \end{cases} \]  

(A1)

where \( u_{BD} \) and \( u_{FD} \) are for forward and backward difference, respectively. The second-order derivative approximations using forward and backward difference schemes are:

\[ \frac{\delta u_{FD}}{\delta x} = -u(x + 2\Delta) + 4u(x + \Delta) - 3u(x) - \frac{\partial u}{\partial x} \]

\[ = -\Delta^2 \frac{\partial^2 u}{\partial x^2} - \Delta^3 \frac{\partial^4 u}{\partial x^4} - \frac{7\Delta^4 \partial^6 u}{60 \partial x^6} + \ldots \]  

(A2)

\[ \frac{\delta u_{BD}}{\delta x} = \frac{3u(x) - 4u(x - \Delta) + u(x - 2\Delta)}{2\Delta} - \frac{\partial u}{\partial x} \]

\[ = -\Delta^2 \frac{\partial^2 u}{\partial x^2} + \frac{3\Delta^4 \partial^4 u}{60 \partial x^4} - \frac{7\Delta^4 \partial^6 u}{60 \partial x^6} + \ldots \]  

(A3)

Therefore, the error for the upwind scheme can be expressed in a single equation as given below:

\[ e = \frac{\delta u}{\delta x} = -u \frac{\Delta^2 \partial^2 u}{\partial x^2} + u \frac{\Delta^3 \partial^4 u}{4 \partial x^4} - \frac{7\Delta^4 \partial^6 u}{60 \partial x^6} + \ldots \]  

(A4)

**A.1. Fourier analysis of numerical error**

Fourier expansion of the velocity field and associated derivative is:

\[ u(x) = \sum \bar{u} e^{ikx}, \]

\[ \frac{\partial u}{\partial x} = \sum ik\bar{u} e^{ikx} = \sum \hat{D}_k e^{ikx}, \]

(A5)

(A6)

where \( \hat{D}_k \) are the Fourier components of the exact velocity derivative. The Fourier representation of error in the convection term is:

\[ \hat{e} = \hat{u} * \frac{\delta u}{\delta x}, \]

(A7)

where * represents convolution. The Fourier component of the forward and backward difference schemes are computed as follows:

\[ \frac{\delta u_{FD}}{\delta x} = \frac{1}{2\Delta} \sum ik\bar{u} e^{ik(2\Delta + k^2\Delta - 3)} \]

\[ = \sum ik\bar{u} \left[ \frac{\sin(k\Delta)}{k\Delta} \right] e^{ikx} \]

\[ + i \left[ \frac{\cos(k\Delta) - 1}{k\Delta} \right] \]

\[ \Rightarrow \hat{D}_{FD} = \hat{D}_k \left[ \frac{\sin(k\Delta)}{k\Delta} \right] e^{ikx} + \left[ \frac{\cos(k\Delta) - 1}{k\Delta} \right] e^{ikx} \]

(A8)

\[ \frac{\delta u_{BD}}{\delta x} = \frac{1}{2\Delta} \sum ik\bar{u} e^{ik(3 + k^2\Delta - 4e^{-ik\Delta})} \]

\[ = \sum ik\bar{u} \left[ \frac{\sin(k\Delta)}{k\Delta} \right] e^{ikx} - i \left[ \frac{\cos(k\Delta) - 1}{k\Delta} \right] e^{ikx} \]

\[ \Rightarrow \hat{D}_{BD} = \hat{D}_k \left[ \frac{\sin(k\Delta)}{k\Delta} \right] e^{ikx} - i \left[ \frac{\cos(k\Delta) - 1}{k\Delta} \right] e^{ikx} \].

(A9)

(A10)
The Fourier components of the error in derivative calculations are:

\[
\frac{\delta u}{\delta x}^{FD}(k) = \hat{D}_e - \hat{D}_F = -\frac{(\cos(k\Delta) - 1)^2}{\Delta} + ik \left[1 - \frac{\sin(k\Delta)}{k\Delta}(2 - \cos(k\Delta))\right]; \quad (A11)
\]

\[
\frac{\delta u}{\delta x}^{BD}(k) = \hat{D}_e - \hat{D}_B = \frac{(\cos(k\Delta) - 1)^2}{\Delta} + ik \left[1 - \frac{\sin(k\Delta)}{k\Delta}(2 - \cos(k\Delta))\right]. \quad (A12)
\]

Thus, the error equation for both \(u \geq 0\) and \(u < 0\) for the upwind scheme is:

\[
\dot{e} = -|\dot{u}| \ast \frac{(\cos(k\Delta) - 1)^2}{\Delta} + \dot{u} \ast ik \left[1 - \frac{\sin(k\Delta)}{k\Delta}(2 - \cos(k\Delta))\right]. \quad (A13)
\]

It must be noted that the real component of the error in the derivative calculation is due to the even derivative terms. Thus, even derivative terms need to be multiplied by the absolute value of the velocity, consistent with the Taylor series expansion analysis above.