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Large-Eddy Simulations Using High-Order Finite Volume Methods with the Stretched-Vortex Subgrid-Scale Model

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As large-eddy simulation is applied to increasingly complex flows, methods of error reduction and controlling computational cost must correspondingly improve. High-order methods are required for resolving critical physics and must be coupled with accurate subgrid-scale models and wall-models. Within this study, the stretched-vortex subgrid-scale large-eddy simulation model is combined with numerical stabilization in the form of the piecewise-parabolic limiter and high-order upwinding to effectively simulate high-Reynolds number flows. Explicit control of the scale at which the subgrid-scale model is computed allows numerically regularized algorithms to accurately simulate large-scale turbulence features that would otherwise be negatively affected by the numerical regularization tested within the current study.

I. Introduction

Very high-Reynolds number flows occur widely in aerospace applications. Experimentally seeking fundamental understanding of such flows is often curbed by the requirements for state-of-the-art facilities that provide well controlled environments and high-resolution spatio-temporal data acquisition systems. Computationally investigating such flows, while constrained by the availability of computing resources, is greatly advanced by the ever-increasing capability of high performance computing (HPC) technologies. As such, large-eddy simulation (LES) has become a practical approach for computational fluid dynamics (CFD) modeling of engineering flows at low- and moderate-Reynolds numbers. However, LES of high-Reynolds number flows still faces a number of challenges.

1) The reliance on and importance of the subgrid-scale (SGS) model significantly increases for high-Reynolds number flows.
2) The interaction of the LES model (including SGS model) with a high-order CFD algorithm becomes intricate and quantifying its impact on predictions requires a detailed understanding of the numerical regularization techniques utilized and the true physics.
3) The influence of adaptive mesh refinement on the LES model needs to be accounted for dynamically.

Practical aerospace applications and HPC are driving CFD algorithms to higher-order accuracy and solution-adaptivity for computational efficiency. Nevertheless, for applications of high-order CFD algorithms to high speed flows, many numerical regularization techniques are employed (e.g., limiters) for stability purposes. These algorithmic components inevitably introduce numerical errors or artificial effects on predictions. If not fully understood, these effects can conceal the true physics. Previous research has highlighted the extent to which the numerical solver affects LES solutions [1].

In order to obtain truly meaningful LES solutions, all components in the modeling system, including the spatial discretization schemes, the numerical regularization methods, any LES and SGS models, as well as any adaptive grids, must be used in a self-consistent and mathematically compatible manner. Recent research has shown that simulations using numerical regularization in addition to turbulence models can provide results that are dominated by the numerical regularization [2]. Even using high-order discretizations and complex numerical regularization machinery, these simulations can still show an over prediction in

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well-resolved kinetic energy. Figure 1 presents such an example where the well-resolved kinetic energy (around $\kappa = 10$) is over-predicted by a fifth-order finite-volume scheme using the piecewise parabolic method (PPM) when compared with the experimentally observed kinetic energy [2, 3]. We conjecture that this particular

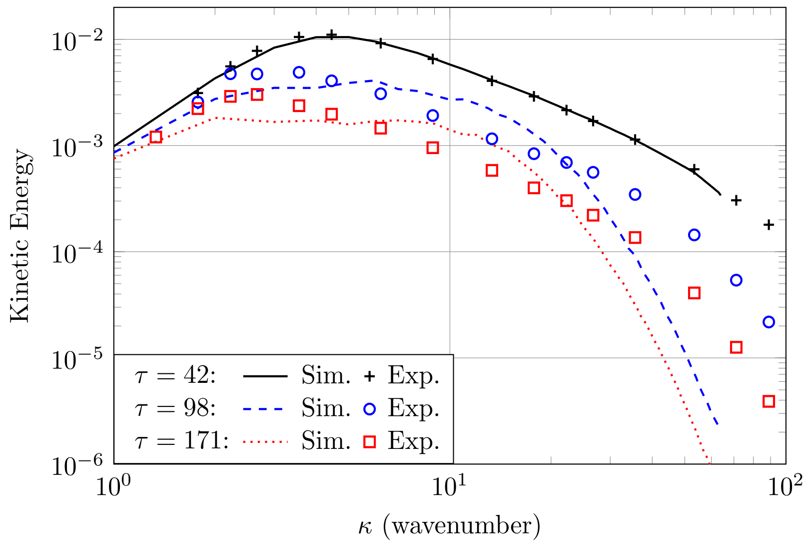


Fig. 1 A comparison of the numerical turbulent kinetic energy spectrum, obtained by using a fifth-order finite-volume scheme with the PPM limiter on a 128^3 grid [2], and the experimentally observed turbulent kinetic energy spectrum [3], for decaying homogeneous isotropic turbulence of $\mathbf{Re}_L = 10400$

phenomenon may be induced by the mismatch of the assumed scales of the turbulence model and the numerical regularization methods. In general, numerical regularization suppresses the smallest represented features leaving only the resolved flow gradients untouched. However, many SGS turbulence models rely, in various ways, on the smallest represented scales and their gradient fields for proper operation. If the SGS turbulence model is also viewed as a regularization technique for turbulent flows, it naturally is expected that both the turbulence models and the standard numerical regularization techniques operate at the same scales. Nevertheless, the major difference is that traditional numerical regularization methods are much stronger than traditional turbulence models since the former are designed for maintaining strict numerical stability. This is particularly true in the use of high-order numerical schemes for simulating flows with strong, under-resolved gradients (e.g. high-Reynolds number turbulent flows). Suppose the smallest representable gradients are essentially removed after a numerical regularization is applied. The turbulence model will no longer have a feature upon which to act in order to aid the flow evolution. The resulting simulation quality fundamentally depends on the underlying interaction between the SGS model and the numerical regularization and only a compatible application of the two can lead to a meaningful solution.

The present study aims to investigate the combination of the stretched-vortex (SV) SGS model and several numerical regularization techniques. Specifically, we focus on delineating this connection using the inviscid Taylor-Green vortex problem. In the limit of infinite-Reynolds number, this case presents challenges to numerical algorithms and thus is well-suited for testing regularization via numerical stabilization methods and/or physical models. The SGS model is applied at multiple scales of resolution in order to determine whether or not the model can aid the flow evolution even in the presence of numerical regularization. In this manner, it is observed that if the SGS turbulence model is applied at the scale of the effective numerical filter (considering only the discretization and traditional regularization techniques), the algorithmic system becomes self-consistent.

II. Computational Framework

Throughout this study, the equations governing compressible turbulent flows are considered [2, 4]. The filtered LES governing equations require some form of closure in order to model filtered nonlinear quantities in terms of the individually filtered, linear components. Throughout the present study, the stretched-vortex subgrid-scale model closes both the filtered momentum and energy conservation equations through the use of a structural model [5–7].

A. Stretched-Vortex Subgrid-Scale Model

Briefly, the SV SGS model was developed from an assumption that the smallest scales in high Reynolds number, turbulent flows are universal in nature. It is assumed that the subgrid turbulent field consists of vortices being stretched by resolved-scale velocity gradients [8]. These stretched-vortices dissipate resolved-scale kinetic energy through the locally increased viscous dissipation brought about by stretching and rotation. This model is well developed and details can be easily found in literature [6, 7, 9–11].

The current study investigates the effect of computing the SGS model components at a larger length scale than that of the mesh. As the SGS kinetic energy estimate is the dominating scaling-factor for the model, the SGS kinetic energy is computed from a coarsening (or filtering) of the data on the mesh and then interpolated to the resolution of the original mesh. Within an algorithmic framework that is capable of adaptive-mesh-refinement (AMR) such as is used in this study, this process of computing the coarse SGS kinetic energy estimate and then interpolating to the original resolution is achieved naturally through the AMR data hierarchy and built-in interpolation operators.

This methodology of computing the SGS kinetic energy estimate at a coarser mesh scale is different from typical explicit filtering methods. Within the framework of traditional explicit filtering, all nonlinear terms are filtered after being computed from filtered data. However, in the context of this particular study, only the SGS kinetic energy is fully computed at a larger scale and then interpolated to the desired mesh resolution.

Throughout this study, the coarsening factor for the SGS kinetic energy estimate computation is a power of two. The coarsened length-scale is denoted by $\Delta_f = n\Delta x$, where $n = 1, 2, 4$.

B. Numerical Algorithm

All results presented in this study are obtained using the FVM algorithm, Chord [12–16], which is built upon Chombo [17]. Chord solves the system of governing equations for transient, compressible, turbulent, reacting and non-reacting fluid flows with complex geometry. It has been designed for achieving superior accuracy and performance for turbulence and combustion simulations on modern high-performance computing architecture. For non-discontinuous flows, Chord is spatially and temporally fourth-order accurate [12–16]. For flows with strong discontinuities (e.g. shock or detonation waves), stability is achieved through the use of the piece-wise parabolic method (PPM) [18, 19] limiter. The solution is temporally evolved with the standard four-stage Runge-Kutta method.

Chord is capable of different levels of turbulence modeling, i.e., unsteady Reynolds-averaged Navier-Stokes (URANS) (using the Spalart-Allmaras model), LES (using the stretched-vortex model), or direct numerical simulation (DNS). Additionally, Chord features AMR in space and subcycling in time, accommodates complex geometry while preserving free-stream conditions using generalized coordinate transformations, and scales to at least 1×10^5 cores.

C. Data Processing

Finally, we note the method for data processing. Mean and unsteady flow variables are processed in accordance with the numerical method used to generate the data-set. For example, data produced with Chord's fourth-order finite volume scheme is post-processed using fourth-order derivatives and the convolution-deconvolution process for converting between cell-averaged values and cell-centered values[19]. Additionally, kinetic energy spectrum are computed with FFTW using cell-centered values.

III. Inviscid Taylor-Green Vortex

The inviscid Taylor-Green vortex problem provides an excellent test case for analyzing the interaction between various algorithmic components such as discretization, numerical regularization (e.g. limiting), and turbulence models. In many ways, it reflects various characteristics of the most challenging engineering problems today. There is no known solution as to how the problem should behave as time evolves towards infinity. Additionally, the problem is representative of very-high-Reynolds number turbulence and has a tendency to break numerical algorithms that lack some form of numerical stabilization. An added benefit that is missing in most practical engineering problems is that the problem is periodic and, as such, does not require treatment of boundary conditions.

Due to the nature of the problem, it is known that the total kinetic energy of the problem (the combination of the resolved and unresolved components) must be conserved. However, with a discrete numerical method, the resolved kinetic energy will certainly not be conserved over the entire simulation time. As the large scale vortices induce smaller vortex formation, the resolved kinetic energy will transfer to unresolved scales. Unless the SGS turbulence model can account for the unresolved kinetic energy, the algorithm will view this unresolved kinetic energy as nothing more than resolved kinetic energy dissipated into internal energy.

All of the LES results presented were run on 64^3, 128^3, and 256^3 Cartesian meshes. The target coarsening length for all of the results presented that use the SV SGS model was such that the equivalent mesh scale would be 64^3.

The initialization for the Taylor-Green vortex is performed in a fully periodic cube of side-length D using the initial condition

$$u = -U_0 \sin\left(\frac{n\pi x}{D}\right)\cos\left(\frac{n\pi y}{D}\right)\sin\left(\frac{n\pi z}{D}\right) \tag{1}$$

$$v = U_0 \cos\left(\frac{n\pi x}{D}\right)\sin\left(\frac{n\pi y}{D}\right)\sin\left(\frac{n\pi z}{D}\right) \tag{2}$$

$$w = 0 \tag{3}$$

$$p = p_0 + \frac{\rho_0 U_0^2}{16}\left(\cos\left(\frac{2n\pi x}{D}\right) + \cos\left(\frac{2n\pi y}{D}\right)\right)\left(\cos\left(\frac{2n\pi z}{D}\right) + 2\right) \tag{4}$$

$$\rho = \frac{p}{RT_0} = \frac{p\rho_0}{p_0} \tag{5}$$

where the number of vortices in the domain in any given direction is denoted by n. The mean velocity is zero while the velocity fluctuation magnitude is given by U_0. The Mach number is 0.1 and the Prandtl number is 0.71. The time-varying results are presented with respect to a non-dimensional, characteristic time, τ. The characteristic time, τ, is defined as

$$\tau = t\frac{U}{L}\ . \tag{6}$$

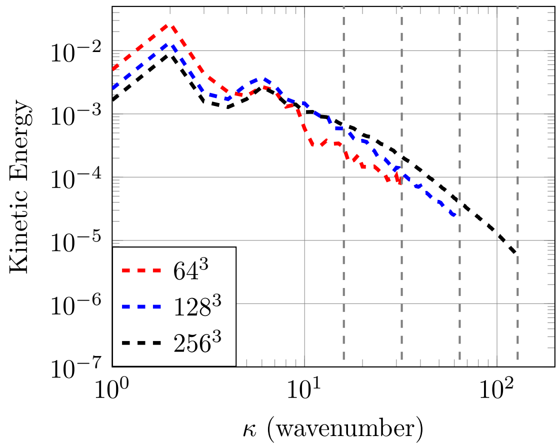
The Taylor-Green vortex problem fully develops turbulence by $\tau \approx 10$. All of the results presented in this study are sampled at $\tau = 20$.

IV. Results and Discussion

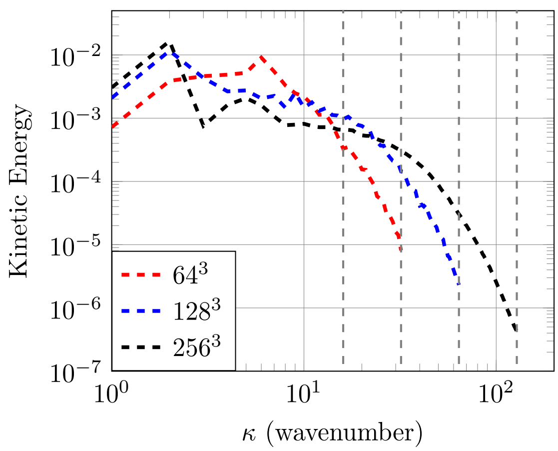
The inviscid Taylor-Green vortex was run with the original SV SGS model and a set of numerically regularized schemes that do not utilize the SV SGS model. The results of these tests, sampled at $\tau = 20$, are presented in Figure 2.

As is evident in all subfigures in Figure 2, no method shows consistency in the behavior of the well-resolved energy scales. It can be observed that the fourth-order SV scheme shows the most consistency in the mid-range energy scales, while the fifth-order SV scheme shows the most consistency over the most well-resolved energy scales. However, the results certainly leave much to be desired. One would hope that some amount of grid-convergence would be reach for the largest scales and that the schemes would eventually agree with one another with enough mesh resolution. If this agreement could be reached, it would be reasonable to hope that the truthfulness of the overall algorithmic framework could be evaluated and changes to models or discretizations could be made as necessary.

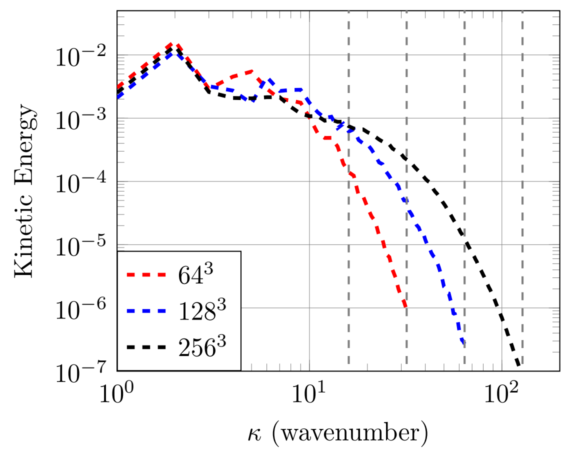
The results using the coarsened SGS kinetic energy estimate are presented in Figs. 3 - 4 with inter-scheme and extra-scheme comparisons separated. Figure 3 presents the equivalent of Figure 2 for each method utilizing the stretched-vortex model. It is apparent that each of the methods presented in Figure 3 display nearly identical results for the largest scales when the 128^3 and 256^3 meshes use the SGS kinetic energy computed on a 64^3 mesh. While a result from a 512^3 mesh using the turbulence model computed at a 64^3 resolution is



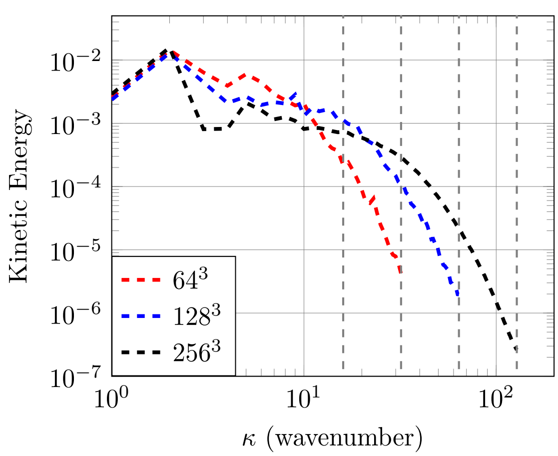
(a) Fourth-order SV



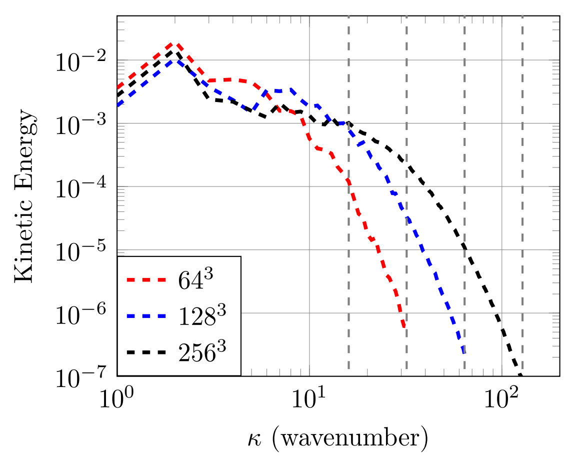
(b) Fifth-order



(c) Fifth-order SV

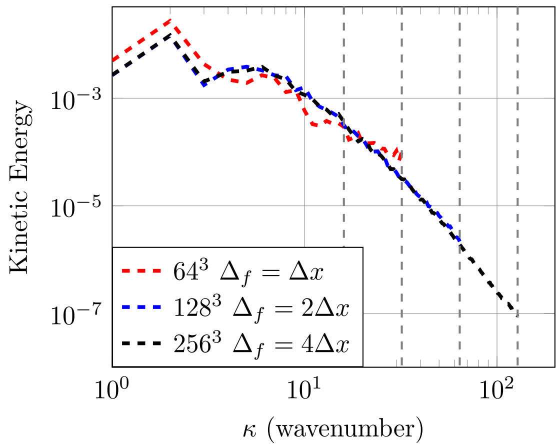


(d) Fifth-order PPM

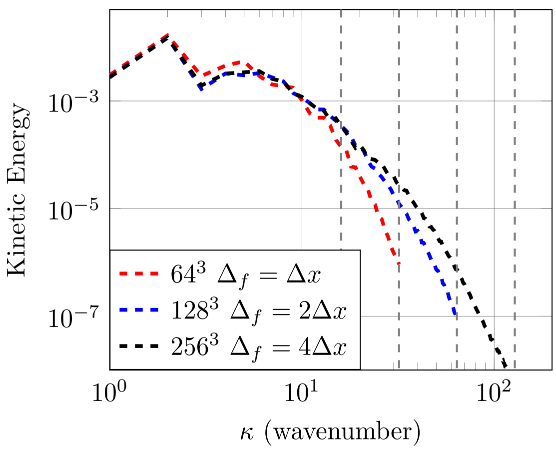


(e) Fifth-order SV PPM

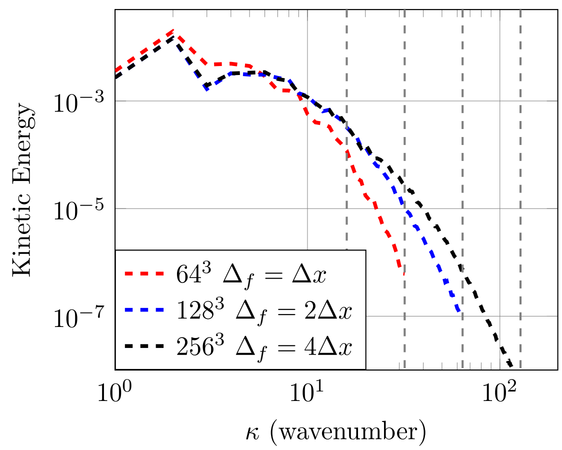
Fig. 2 Inviscid Taylor-Green vortex kinetic energy spectrum using no coarsening of the SGS kinetic energy estimate, $\tau = 20$



(a) Fourth-order SV

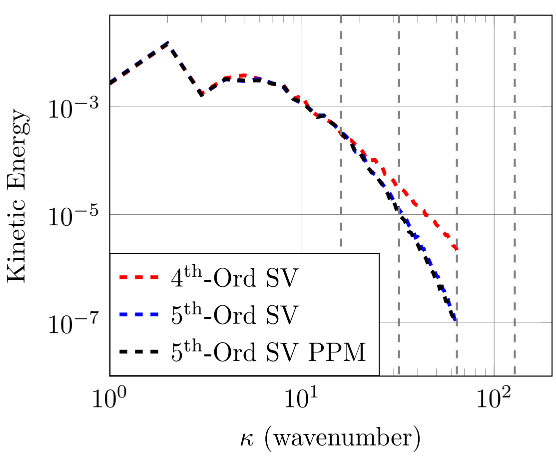


(b) Fifth-order SV

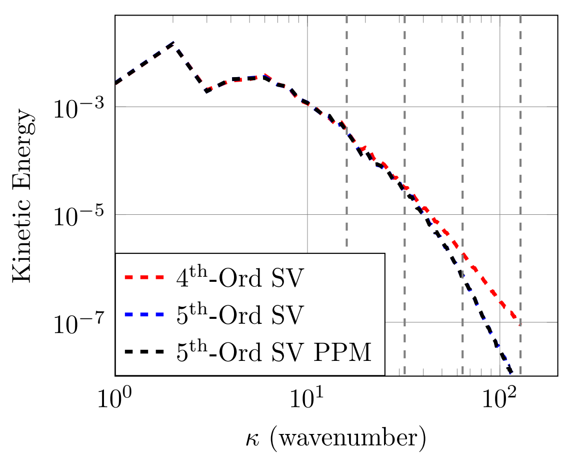


(c) Fifth-order SV PPM

Fig. 3 Energy spectrum with the coarsened SGS energy estimate, $\tau = 20$



(a) 128^3 Mesh, $\Delta_f = 2\Delta x$



(b) 256^3 Mesh, $\Delta_f = 4\Delta x$

Fig. 4 Energy spectrum with the coarsened SGS energy estimate, $\tau = 20$

not presented, it is still believed that the results that were obtained are displaying grid-independence of the largest scales.

What is perhaps even more convincing and encouraging are the results presented in Figure 4 displaying the comparison between varying schemes. These results demonstrate that, even when combined with numerical regularization, the coarsened form of the SV model implementation displays nearly identical results between schemes. This lack of difference between the fourth-order, fifth-order, and fifth-order PPM schemes all using the SV model is most pronounced in Figure 4b where the 256^3 mesh is used with a coarsening ratio of four for the turbulence model computation. In all simulations, it was noted that a coarsening ratio of four was the maximum necessary to achieve nearly identical solutions between the schemes. Although the results with a coarsening ratio of eight are not presented, they showed almost identical results as compared to the simulations utilizing a coarsening factor of four.

V. Conclusion

With the way modern high-performance computing architectures have evolved and the increasing demand on solution fidelity that comes from practical engineering design, the need for high-order accurate simulations of high-Reynolds number flows with complex physics will be a continual challenge that the CFD community must meet for the foreseeable future. As high-order algorithms and complex physics models are combined, the mathematical consistency of these systems and the compatibility of each component are required in order to achieve the highest-fidelity possible.

In this study, it is demonstrated that the stretched-vortex large-eddy simulation subgrid-scale model can be effectively used with numerical regularization techniques such as upwinding and interpolation limiting if the turbulence model is applied to the system in a manner consistent with the rest of the algorithm. As the numerical regularization increases the algorithmic effective-filter width, the turbulence model must be applied at a larger length scale in order to achieve results that provide grid-independence of the largest scales.

Additionally, it was found that computing the SGS kinetic energy estimate at a coarser scale provided a decrease in computational effort. This method of turbulence model calculation naturally fits into multi-scale frameworks such as adaptive mesh refinement and multigrid methods. With such frameworks, the benefits of coarse-scale computations of the turbulence model are fully realized.

Near-term studies will extend this result to wall-modeled LES simulations of high-speed reacting flows. It is expected that the benefits of a coarsened SGS kinetic energy calculation will carry over to wall-modeled simulations and that phenomenon frequently encountered in such simulations (e.g. log-layer mismatch) will naturally be corrected.

VI. Acknowledgment

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