LES modeling of scalar transport based on high-order discontinuous finite-element method: Assessment of implicit LES and scalar variance modeling

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I. Introduction

The modeling of turbulent scalar transport processes is important in multi-physics flow problems, such as reactive flow, pollutant dispersion in the atmosphere, and drug delivery through blood flows. Enabling accurate predictions of these flow phenomena requires reliable models to describe scalar transport for turbulent flow condition. In the context of large-eddy simulation (LES), models typically account for effects of the subgrid-scale (SGS) behavior on the resolved scalar/velocity fields. Several previous studies are concerned with the LES modeling of scalar transport, for example, in combustion applications or geophysics flows.

In regard to LES-modeling, numerical algorithms often interfere with the modeling performance. The numerical basis for supporting the modeling in previous works are either pseudospectral schemes or finite difference/finite volume schemes. As such, they are either not applicable or constrained by second-order accuracy when complex geometries for practical applications are considered. For practical LES, recently developed discontinuous finite element methods (in particular discontinuous Galerkin, DG) shows potential for application to LES by providing high-order accuracy, improved convergence, and lower numerical diffusion. Further, studies have shown that implicit LES based on DG yields improved predictions compared to classic FD/FV based LES, even with coarser mesh-resolution. However, efforts for developing or assessing LES for DG are still concentrated on the modeling of the flow-field characteristics. The compatible numerical treatment for scalar-transport modeling has so far not been systematically examined.

Motivated by the increasing interest in the LES modeling for scalar transport, the present study aims to assess the performance of DG for the prediction of scalar transport. This assessment is conducted through the systematic comparison with state-of-the-art LES techniques based on a 2nd-order FD scheme and dynamic modeling strategy. As counterpart, the model-free treatment is retained for the DG scheme. The output obtained from this setting is intended to shed some insight on the model development for DG. For scalar transport, the quantities of interest include the PDF, scalar variance and energy spectrum of the resolved scalar field; special attention is paid to assess the modeled subfilter scalar variance, which is particularly important for accurately incorporating combustion models.

The rest of the paper is structured as follows: The mathematical model and numerical method will be introduced in Sec. II. Sec. III provides the flow configuration, followed by the generation of the corresponding DNS databased in Sec. IV. The LES results and discussions will be given in Sec. V. The paper finishes by drawing conclusions in the last section.

II. Numerical Method

II.A. Governing Equations

We consider the compressible Navier-Stokes equations with one conserved scalar:

$$\partial_t \rho + \partial_i (\rho u_i) = 0$$  \hspace{1cm} (1a)

$$\partial_t (\rho u_i) + \partial_j (\rho u_j u_i + p \delta_{ij}) = \partial_j \tau_{ij}$$  \hspace{1cm} (1b)

$$\partial_t (\rho e) + \partial_j (u_j (\rho e + p)) = \partial_j (u_i \tau_{ij} - q_j)$$  \hspace{1cm} (1c)

$$\partial_t \rho Z + \partial_i (\rho Zu_i) = -\partial_j j_i$$  \hspace{1cm} (1d)
To develop a discontinuous Galerkin scheme, we start by writing the Navier-Stokes equations in index form:

\[ \mathbf{\tau}_{ij} = \mu(\partial_i u_j + \partial_j u_i) - \delta_{ij} \frac{2}{3} \mu \partial_m u_m, \]  
\[ q_i = -\kappa \partial_i T, \]  
\[ j_i = -\alpha \partial_i Z, \]

in which the involved parameters are dynamic viscosity \( \mu \), thermal conductivity \( \kappa \), and mass diffusivity \( \alpha \).

This set of equations is closed by the ideal gas law,

\[ p = (\gamma - 1) \left( \rho e - \frac{\rho u \cdot u}{2} \right) \]

which relates pressure with internal energy; \( \gamma \) is the ratio of specific heat capacity, set to 1.4 in this study.

For LES, the governing equations, Eq. (1), are convolved with a certain low-pass filter kernel, to obtain a filtered version. Since we primarily focus on the implicit LES technique, solutions obtained by directly discretizing Eq. (1) is equivalent to the filtered LES variables. Thereby, in the present study, we are not distinguishing both.

### II.B. Discontinuous Galerkin Discretization

To develop a discontinuous Galerkin scheme, we start by writing the Navier-Stokes equations in index form:

\[ \partial_t U_j + \partial_k F^c_{kj} - \partial_k F^v_{kj} - S_j = 0, \]

where \( U_j \) refers to the \( j \)th component of the conservative state vector, and \( F^c_{kj} \) and \( F^v_{kj} \) are the corresponding \( j \)th component of the inviscid and viscous flux along the \( k \)th spatial dimension. \( F^c_{kj} \) is a non-linear function of the full state vector, and \( F^v_{kj} \) can be linearized with respect to the gradients of the conservative variables.

A spatial discretization is then obtained by partitioning the computational domain \( \Omega \) into a set of non-overlapping elements \( \{ \Omega_e \} \) with boundaries \( \partial \Omega_e \). Then, we consider the finite-dimensional functional space \( V_h \), with

\[ V_h^p = \{ \phi \in L^2(\Omega_e), \phi \in P^p(\Omega_e) \forall \Omega_e \in T_h \}, \]

where \( T_h \) is the mesh partition, and \( P^p \) denotes the space of polynomial functions of degree \( p \). The solution to \( U_j \) is approximated by the polynomial space as:

\[ U^h_j(t, \mathbf{x}) = \sum_{q=1}^{N_p} \tilde{U}_{j,q}(t) \phi_q(\mathbf{x}), \]

where \( \tilde{U}_{j,q}(t) \) is the time-dependent coefficient of the \( q \)th expansion term. A variational formulation is then obtained by multiplying Eq. (4) by a test function \( \phi \) and integrated over each element,

\[ \int_{\Omega_e} \phi_t \tilde{U}_{j,q}(t) + \int_{\Omega_e} \phi_i \partial_i \tilde{U}_{j,q} + \int_{\Omega_e} \phi_i \partial_i \tilde{F}^c_{kj} + \int_{\Omega_e} \phi_i \partial_i \tilde{F}^v_{kj} - \int_{\Omega_e} \phi_i S_j = 0. \]

In this equation, the first term on the left-hand-side (LHS) is the mass matrix and the fourth term is element-local and can be directly evaluated using quadrature rule.

The second term is the advection term, and is treated by partial integration:

\[ \int_{\Omega_e} \phi_t \partial_i \tilde{F}^c_{kj} + \int_{\partial \Omega_e} \phi_i \tilde{F}^c_{kj} \partial_n \mathbf{n} + \int_{\partial \Omega_e} \phi_i \tilde{F}^v_{kj} \partial_n \mathbf{n} \]

where \( \mathbf{n} \) is the outward pointing normal on \( \partial \Omega_e \). On \( \partial \Omega_e \), the notation \( (\cdot)^+ \) and \( (\cdot)^- \) refers to the quantities taken from the interior and exterior of element \( \Omega_e \), respectively. The elements are essentially tied to each other through the numerical flux \( \tilde{F}^e_{kj} \), which is here discretized using a local Lax-Friedrichs flux.

The viscous-diffusive flux, appearing as the third term on the LHS of Eq. (7), includes second-order derivatives. This term is linearized and expressed in terms of the conserved state-variables:

\[ \tilde{F}^v_{kj} = A_{klji} \partial_l U_i \]

with index \( i \) and \( l \) referring to the state-vector and spatial dimension, respectively. The fourth-order tensor \( A_{klji} \) accounts for the differentiation of the viscous flux with respect to \( \partial_i U_i \). The discretization of the viscous term follows the symmetric interior penalty method. \( \text{(9)} \)
II.C. Consistent dynamic modeling approach for subfilter variance

An important component of this work is to assess the prediction of subfilter scalar variance using the DG scheme. We utilize the dynamic procedure for modeling the subfilter scalar variance, which dates back to the original work by Pierce and Moin.\(^9\) To explain this modeling approach, we start from the definition of the subfilter variance \( \widetilde{Z'}^2 \):

\[
\widetilde{Z'}^2 
\equiv \int \left( Z(x') - \widetilde{Z}(x) \right)^2 G(x' - x) \, dx' = \widetilde{Z'}^2 - \widetilde{Z}^2 .
\]  

(10)

Based on this definition, a transport equation for \( \widetilde{Z'}^2 \) can be derived analytically:

\[
\frac{D \widetilde{Z'}^2}{Dt} = \frac{\partial}{\partial x_i} \left( D \frac{\partial \widetilde{Z'}^2}{\partial x_i} \right) - \left( 2D \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial \widetilde{Z}}{\partial x_i} - 2D \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial \widetilde{Z}}{\partial x_i} \right) 
\]

\[
- \frac{\partial}{\partial x_i} (u_i \widetilde{Z}^2 - \bar{u}_i \bar{Z}^2) + 2 \bar{Z} \frac{\partial}{\partial x_i} (u_i \bar{Z} - \bar{u}_i \bar{Z}) ,
\]

(11)

in which the term (a) refers to the scalar dissipation rate due to subgrid scales, while the term (b) exhibits the redistribution and production by SGS correlations between velocity and scalar-energy (squared scalar) and between velocity and scalar. In the following derivation, the dissipation and production terms are denoted as \( \Psi \) and \( \epsilon \), respectively. Both terms involves SGS terms which invoke closure issues. The dissipation term is commonly linked to a mixing time scale \( \tau_z \), with which:

\[
\epsilon \sim \widetilde{Z'}^2 / \tau_z .
\]

The production term is modeled using an eddy-diffusivity model:

\[
\Psi = D_t \frac{\partial \bar{Z}}{\partial x} \frac{\partial \bar{Z}}{\partial x} .
\]

in which we implicitly assume that the molecular diffusion effects are negligible compared to the turbulent diffusion effect. To finalize the elaboration, we need to invoke the so-called local equilibrium assumption that reads \( \Psi = \epsilon \). With this, a simple algebraic closure model for \( \widetilde{Z'}^2 \) is obtained:

\[
\widetilde{Z'}^2 = C_v \Delta^2 \frac{\partial \bar{Z}}{\partial x} \frac{\partial \bar{Z}}{\partial x} ,
\]

where \( \Delta \) is the grid size and the parameter \( C_v \) is model-parameter that needs to be determined. In practice, \( C_v \) is often determined by applying a test filter and constructing the Leonard term:

\[
\widetilde{Z'}^2 - \widetilde{Z'}^2 = \bar{Z}^2 - \bar{Z}^2 = C_v \left( \Delta^2 |\nabla \bar{Z}|^2 - \Delta^2 |\nabla Z|^2 \right) ,
\]

(12)

where \( \cdot \) refers to a quantity that is filtered by the test filter. With this relation, the term \( C_v \) can be computed as a pointwise value subject to temporal updates. The advantage of this model is that it remains parameter-free. Balarac et al.\(^13\) proposed a modification to this approach based on a Taylor-expansion on the left side. In their modification, only the first term on the right-hand side is retained. This simplification leads to considerable improvement of the model performance. Following this idea, we utilize the following form for the evaluation of \( C_v \):

\[
C_v = \frac{\bar{Z}^2 - \bar{Z}^2}{\Delta^2 |\nabla \bar{Z}|^2} .
\]

(13)

The key issue for enabling this procedure in DG is how to propose the test filter and conduct the filtering operation. One natural option for DG is to utilize a subspace as a test filter and use least-square projection for computing test-filtered quantities related to this subspace filter. This treatment is the essential component of the proposed approach for enabling the LES modeling for DG scheme.
II.D. Summary of solver details

The numerical technique developed based on DG approach will be compared to that of a widely used LES solver-3DA,\textsuperscript{14} which was developed based on a second-order FD scheme. Both numerical techniques differ in several aspects. First, the two solvers solve different sets of governing equations. The DG solver solves the fully compressible Navier-Stokes equations, as introduced in Eq. (1), which the 3DA solver solves the incompressible Navier-Stokes equations. As for the incompressible version, the Poisson system needs to be solved along with the moment equation and the scalar-transport equation, to enforce the divergence-free constraint of the flow field. Second, the two solvers, which are built on completely different numerical schemes, have different orders of accuracy. In theory, the DG solver is able to reach arbitrarily high order (although we use the fourth-order scheme throughout this study), while the 3DA solver has second-order accuracy. Another aspect distinguishing both is the LES capability. For the DG solver, the implicit LES strategy is employed and the numerical dissipation inherent in the Riemann flux functions like SGS dissipation, while in 3DA the dynamics Smagorinsky model\textsuperscript{15} is used as the SGS closure model, with the extension to account for the SGS effects on scalar transport.\textsuperscript{8} For the modeling of subfilter scalar variance, a test filter needs to be implemented. For this, 3DA uses a box filter defined on physical space, while DG utilizes a projection operator that projects the local solution to a \((p-1)\)-order polynomial space using least-square. Here \(p\) refers to the polynomial space for representing resolved solution fields. More details related to the two solvers are listed in Table 1.

<table>
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<th>Table 1: Summary of numerical techniques</th>
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III. Problem configuration

In this study, we consider the problem of scalar transport in canonical decaying turbulence. A three-dimensional periodic domain is employed with a length \(L = 2\pi\) in each direction. The turbulence Reynolds number, \(\text{Re}_\lambda = \lambda u' / \nu\), defined with respect to the Taylor scale \(\lambda\), is 40. The Prandtl and Schmidt numbers both are set to 0.7. The Mach number is set to 0.1 for the DG-based compressible solver in order to retain the incompressible flow condition. The initial field for the fluctuation velocity, \(u'\), is specified using a pseudo energy spectrum:

\[
E_u(k) \sim k^4 \exp(-2k^2/k_0^2), \tag{14}
\]

where \(k_0\) is the most energetic wavenumber, related to \(\lambda\). The eddy turnover time, \(\tau = \lambda/u'\), is set 0.5. As long as an initial value for \(u'\) is specified, the velocity field, as well as the viscosity \(\nu\) can be calculated
according to the above specifications. The Kolmogorov scale is estimated as $0.04L$. For the present study, the spectrum of the initial velocity field is shown in Fig. 1(a). The field for a scalar, $Z$, is initialized using the method proposed by Eswaran and Pope. The key idea of this method is to embed scalar blobs with certain characteristic length in the 3D box. This length scale can be specified on the wavenumber space. For the present study, it is $L/k_z$ with $k_z = 4$ that can be observed in the initial scalar spectrum given in Fig. 1(a). A relatively sharp scalar interface is retained so that the scalar PDF initially retains a double-Delta shape, as observed in Fig. 1(b). Further, the initial scalar field is visualized with color contour plot in Fig. 1(c) for providing more intuitive information.

![Energy spectrum of DG-based LES](image1.png)  
(a) energy spectrum of DG-based LES  

![Energy spectrum of FD-based LES](image2.png)  
(b) energy spectrum of FD-based LES  

![Evolution of scalar energy](image3.png)  
(c) evolution of scalar energy  

Figure 1: Initial conditions for the simulations.

## IV. Generation of DNS data

A reliable DNS database needs to be generated as the reference for the assessment of LES performance. Both solvers are employed to generate the DNS database. Although they are developed based on different numerical techniques, it is anticipated that the DNS results shall converge to the same results. To confirm this point, we perform mesh-refinement studies with both solvers, and compare the converged solutions of individual set. The results are shown in Fig. 2. The temporal evolution of the domain-averaged scalar energy does not exhibit noticeable difference among all cases. Therefore, the spectra of scalar energy are examined for comparison of more detailed solution characteristics. In Figure 2(b-d), the spectra are plotted at the end of simulations, $t/\tau = 4$, and up to the wavenumber corresponding to the Kolmogorov scale. From Fig. 2(c), the DG solver is able to obtain a converged solution with $128^3$ resolution, thanks to its high-order accuracy. However, it can be observed in Fig. 2(d) that the results for 3DA on $128^3$ resolution still reveal relatively large discrepancies from these of more refined calculations over the wavenumber range, $2 \leq k \leq 6$. Thereby, the 3DA calculations are executed with two more levels of mesh refinements to ensure convergence. Good agreement on the scalar-energy spectrum is observed between $256^2$ and $384^3$ resolutions. Hence, we consider the latter case as the converged solution from 3DA, which is further compared to the DNS solution obtained by the DG solver. This comparison is given in Fig. 2(b), and we can see excellent agreement between the converged spectra from two different solvers, although they are obtained using completely different numerical techniques.

So far, we have focused on the prediction of scalar-related quantities. The accurate prediction of scalar transport relies on the correct prediction of velocity field. Therefore, the DNS results on turbulent kinetic energy (TKE) are also examined. Figure (3) (a) shows the temporal evolution of TKE and Figure (3) (b) shows the energy spectrum of TKE computed at the end of the simulation. The excellent agreement between the DG prediction and the 3DA prediction is once again observed. In the following, either of the set of DNS prediction can be used as the reference for assessing LES performance. To facilitate the comparison with the following LES results, the DNS database will be filtered with different filter sizes defined by the corresponding LES meshes. Furthermore, the different filtering approaches are applied in the two solvers. For DG-based LES, the DNS data is projected on the LES mesh using an element-wise least-square procedure, while for FD-based LES with 3DA the DNS database is filtered using a box filter on physical space.
V. Assessment of LES predictions

The LES calculations using both solvers are performed on two sets of meshes that include $16^3$ and $32^3$ degrees of freedom, respectively. Sec. V.A discusses the predictions of scalar-related quantities, followed by the discussion of velocity field prediction in Sec. V.B. The performance of predicting subfilter scalar variance is assessed in Sec. V.C.

V.A. Prediction of scalar transport

The resolved scalar energy and the energy spectra of the resolved scalar field, obtained using two different LES techniques, are analyzed and compared. The results are presented in Fig. 4. From both sets of results, the
LES predictions approaches the DNS reference solution as the resolution increases. However, the behaviors of the solutions subject to mesh refinements exhibit substantial differences. For DG-LES, the solution on very coarse resolution (16$^3$) reveals significant energy overshoot, while the result obtained with FD-LES is overly dissipative. As resolution is improved to 32$^3$, DG predicts an evolution of scalar energy very close to the DNS result, as seen in Fig. 4(b). Comparatively, the energy prediction using 3DA still have a large undershoot compared to the DNS reference solution. The solution improvements by refinements are more apparent on the spectra of scalar energy shown in Fig. 4 (b, c). The spectra are examined at the end of simulation, $t/\tau = 4$. In the DG prediction, the energy overshoot spreads over all the resolved wavenumbers in the 16$^3$ case; as the resolution rises to 32$^3$, the DG-LES prediction shows excellent agreement with the DNS reference solution, except for a small amount of energy undershoots in the range close to the cutoff wavenumber. On the contrary, the FD-LES underpredicts the energy almost over all the resolved wavenumbers for both different resolutions. On the refined mesh (32$^3$), the energy level of the lower wavenumbers exhibits a slight increase, while the resolution range extends. The FD-based LES performs slightly better in terms of preserving the decay rate of scale energy at small scales.

Figure 3: Comparison of TKE prediction in the DNS of decaying homogenous isotropic turbulence.

Figure 4: Comparison of the LES results of scalar transport in decaying homogenous isotropic turbulence.
V.B. Prediction of velocity field

The LES predictions of TKE temporal evolution using the both DG and 3DA solvers are shown in Fig. 5. From Fig. 5(a), we can see that the amount of resolved TKE on different LES meshes by both solvers are comparable, although the resolved scalar energy behaves differently (see Fig. 4(a)). The energy spectra of TKE are examined at the end of the simulation, \( t/\tau = 4 \), which are shown in Fig. 5(b) and (c). The two sets of LES results provide very good agreement with the DNS solution. The FD-LES with 3DA leads to slight undershoot of scalar energy over a wide range of wavenumber, say \( 4 \leq k \leq 16 \), but the decay rate along the wavenumber space is well preserved. In contrast, the implicit LES using the DG solver is able to provide better predictions for the TKE at relatively large scales, for example in the range \( 4 \leq k \leq 8 \), but the decay rate at large wavenumber deviates from the DNS data. Given the subtle difference between the two sets of LES predictions, it is difficult to judge whether each one is superior over another. Nevertheless, based on the present result we can claim that the performance of the DG-based implicit LES provides comparable performance to the commonly used explicit FD-LES (at least in the present case).

![Figure 5: Comparison of the LES predictions of TKE in decaying homogenous isotropic turbulence.](image)

V.C. Prediction of subfilter scalar variance

This section focuses on the LES prediction of subfilter scalar variance. Figure 6 shows the evolution of the domain-averaged subfilter variance. It is evident that the FD-LES by the 3DA solver underpredicts the reference magnitude of scalar variance obtained from the filtered DNS data. This observation is consistent with the previous study. Comparatively, the DG scheme provides improved predictions. Furthermore, increase of LES resolution leads to the improvement of the predictive performance for both schemes. Another interesting finding is that the filter for the DG-LES cuts much smaller parts of the energy than the box filter used in the FV-LES. A phase shift is also observed by comparing the different sets of filtered data. In order to examine the detailed characteristics of the predicted subfilter variance, PDFs of both predicted and DNS-filtered variances are compared using the quantile-quantile plots. Since the DG method is built on a variational formulation, the solution presented by piecewise polynomials does not facilitate a point-to-point comparison. Therefore, we consider using the cell averaged variance to form the PDF for comparison. Results for the DG scheme are given in Fig. 7. At different solution times, we observe good agreement between the predicted PDFs and the DNS-filtered PDFs. This set of DG-LES results is compared to that obtained by the FD-LES in Fig. 8. We can see that the deviation of the scalar variance PDF predicted by FD-LES is significantly smaller than that obtained from the filtered DNS data. At different solution times, we can also see the center of the scattered data is biased towards the left-hand side, consistent with the considerable undershoots shown in Fig. 6(b). Compared to the FD-LES approach, the DG-LES improves the predictions on the PDF of subfilter scalar variance, \( \tilde{Z}'^2 \).
VI. Prevention of scalar-energy overshoot

In light of the overshoot of scalar energy observed in Sec. V.A, caution needs to be taken whenever we tend to interpret the under-resolved DG predictions from the LES perspective. In term of LES, the scalar energy is expected to be no larger than the corresponding DNS prediction; in this sense, the DG-LES on the very coarse mesh (16\(^3\)), shown in Fig. 4(a), is not a valid LES prediction. This phenomenon implies that in the DG scheme the inherent dissipation on the resolved scalar field is much less than the physical dissipation provided by the subfilter scale field. Additional dissipation needs to be introduced to the scalar field in order to achieve a valid LES prediction using the DG method. For this, we consider to augment the mass diffusivity of the transport scalar in Eq. (1) with an artificial diffusivity \( \alpha \rightarrow \max\{\alpha, \alpha_{AD}\} \). The magnitude of \( \alpha_{AD} \) is determined through the stability analysis of a linear convection-diffusion equation,
(a) FD-LES, $t/\tau = 1$
(b) FD-LES, $t/\tau = 2$
(c) FD-LES, $t/\tau = 3$

Figure 8: Quantile-quantile comparison of the predicted subfilter scalar variance to that of the filtered DNS data.

which was presented in our previous work. The general formulation reads:

$$\alpha_{AD} = (\beta - 1) \frac{C_1}{C_2} ah,$$

(15)

where $\beta$ is an empirical parameter that varies between 1 and 2, $C_1$ and $C_2$ are functions of polynomial order $p$, $a$ is the characteristic advection speed of the transport equation, and $h$ is the size of DG element. For scalar transport, the characteristic speed is chosen to be the local flow velocity, $a = |u|$. Based on the previous analysis, $C_1$ and $C_2$ are selected to be 19.1 and 173.0, respectively, and the parameter $\beta$ is suggested to be 1.15 for linear cases. With this, we obtain a complete specification for $\alpha_{AD}$, which ensures the solution consistence to the first principle as $h$ goes to zero. The LES with this artificial-diffusivity formulation is carried out using the DG solver. The results are compared to the original DG-LES performed without artificial diffusivity in Fig. 9. We can see that the overshoot in scalar energy on $16^3$ mesh is effectively avoided, and by comparing to the FD-LES results shown in Fig. 4 we also observe that with the artificial diffusion formulation the amount of scalar energy resolved by the DG solver on $16^3$ mesh becomes comparable to that resolved by 3DA on $32^3$ mesh. For the DG results on $32^3$ mesh, the original LES calculation already more or less converges to the DNS reference. In this case, the artificial diffusion formulation preserves the original resolution, and the resolved scalar energy remains unchanged. This confirms that the LES with the artificial diffusivity method is able to revert to the corresponding DNS, if the resolution becomes sufficiently high.

VII. Conclusions

This study performed assessment of DG-based implicit LES technique in predicting scalar transport in a canonical decaying turbulence. A fourth-order DG scheme was employed and compared to the commonly used explicit LES approach built on second-order finite difference scheme. A DNS study was firstly conducted to generate the reference solution for subsequent LES calculations. The LES predictions focused on the resolved scalar energy, the energy spectrum of the resolved scalar field, and the subfilter scalar variance based on a dynamical procedure. Several findings were summarized in the following:

- In terms of DNS calculations, high-order DG scheme provides faster solution convergence than the second-order finite difference scheme.

- In terms of LES, the implicit LES technique built on DG scheme tends to overpredict the scalar energy on highly underresolved LES meshes. In contrast, the explicit LES results obtained from 3DA solver show underprediction for the scalar energy. The latter solution behavior conforms better to the classical concept of large-eddy simulation, while the former solution behavior indicates that the scale-dissipation mechanism in DG is not sufficiently strong compared to that brought physically from the subgrid scales.
when the mesh resolution is very poor. In terms of prediction of turbulent velocity field, the DG-based LES approach provides similar performance to the FD-based explicit LES method.

- For LES modeling of subfilter scale variance, the implicit LES built on the high-order DG scheme shows potential in leveraging prediction quality.

Following up on the assessment, we proposed a novel method to avoid the overshoot of scalar energy in the DG-LES predictions, especially on very coarse meshes. The method augments the physical scalar diffusivity with an artificial diffusivity which vanishes as $h$ decreases. The DG-LES equipped with this artificial-diffusivity approach was compared to the LES with the standard DG scheme. The overshoot of scalar energy was found to be effectively prevented. In future, this assessment of DG-LES technique will be extended to the modeling of reactive scalars in combustion applications. More realistic flow configurations, such as jets and channel flows, will be considered for comprehensive investigations.

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**References**


