Quantitative analysis on implicit large eddy simulation

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I. INTRODUCTION

Large eddy simulation (LES) is proposed to solve the filtered Navier-Stokes equations (NSE) with resolvable turbulent structures above the inertial scale. Static explicit large eddy simulation (eLES) has been widely used in unsteady separated turbulent flows. Different with the eLES, implicit large eddy simulation (iLES) takes the built-in numerical dissipation as the subgrid-scale (SGS) dissipation. Due to the lower computational costs and reasonable performance, iLES has been gradually utilized in LES community.

In the past decades, the finite-volume gas-kinetic scheme (GKS) based on the Bhatnagar-Gross-Krook (BGK) model have been developed systematically for computations from low speed flows to supersonic ones. The GKS presents a gas evolution process from kinetic scale to hydrodynamic scale, where both inviscid and viscous fluxes are recovered from a time-dependent and multi-dimensional gas distribution function at a cell interface. Based on the time-dependent flux, a reliable two-stage framework was provided for developing the high-order GKS (HGKS). In terms of low-Reynolds number turbulent flows, the HGKS has been used as a direct numerical simulation (DNS) tool. The numerical performance (i.e., numerical accuracy, robustness) and computational cost is comparable with the widely-used high-order finite difference method. HGKS also shows advantage in supersonic turbulence studies due to its reliable robustness. HGKS indeed provides a valid tool for the numerical simulation of turbulence, which is much less reported in finite volume scheme.

HGKS has been implemented for the iLES in compressible turbulent flows, i.e., compressible turbulent flow over periodic hills with volumetric Mach number $M_{b}$ = 0.2 and cross-sectional Reynolds number $Re_b$ = 2800. Compared with the key statistical quantities of DNS, we found that iLES outweighs eLES on the exactly same unresolved grids. eLES over-predicts the normalized Reynolds stresses and provides much stronger turbulent fluctuation than that of DNS solution. While, the solutions from iLES agree well with the DNS results, and the over-predicted performance seldom appears. Thus, we speculated that the static explicit LES model may pollute the resolved turbulent structures of low-Reynolds number separated turbulent flows. To shed light on the seemingly abnormal performance, current research conducts the quantitative comparisons between iLES and eLES based on the Taylor-Green vortex benchmark, especially focusing on the numerical SGS dissipation and modeling SGS dissipation.

This paper is organized as follows. After the introduction, HGKS is introduced briefly. Followed by the numerical results and quantitative analysis, the last section presents the conclusion and discussion.
II. FOURTH-ORDER GAS-KINETIC SCHEME

iLES and eLES in compressible Taylor-Green vortex problem are implemented with fourth-order GKS\textsuperscript{14}. GKS is the well-developed finite-volume scheme based on the BGK equation. The three-dimensional BGK equation\textsuperscript{10} reads
\begin{equation}
    f_i + u f_i + v f_j + w f_z = \frac{g-f}{\tau},
\end{equation}
where \( u = (u, v, w)^T \) is the particle velocity, \( f \) is the gas distribution function, \( g \) is the three-dimensional Maxwellian distribution and \( \tau \) is the particle collision time. Chapman-Enskog expansion\textsuperscript{20} provides \( \tau = \mu / p \), where \( \mu \) is the molecular viscosity and \( p \) is the pressure. The collision term satisfies the compatibility condition
\begin{equation}
    \int \frac{g-f}{\tau} \psi d\xi = 0,
\end{equation}
\( N = (5 - 3\gamma) / (\gamma - 1) \) is the internal degree of freedom, and \( \gamma \) is the specific heat ratio.

Taking moments of Eq.(1) and integrating with respect to space, the finite volume scheme can be expressed as
\begin{equation}
    \frac{d(Q_{ijk})}{dt} = \mathcal{L}(Q_{ijk}),
\end{equation}
where \( Q_{ijk} \) is the vector of conservative variables, namely, density \( \rho \), momentum \( \rho u_i \), and total energy \( \rho E \). The operator \( \mathcal{L} \) is defined as
\begin{equation}
    \mathcal{L}(Q_{ijk}) = -\frac{1}{|\Omega_{ijk}|} \sum_{p=1}^{6} F_p(t),
\end{equation}
where control volume \( \Omega_{ijk} = x_i \times y_j \times z_k \) with \( x_i = [x_i - \Delta x/2, x_i + \Delta x/2] \), \( y_j = [y_j - \Delta y/2, y_j + \Delta y/2] \), \( z_k = [z_k - \Delta z/2, z_k + \Delta z/2] \). \( F_p(t) \) is the numerical flux across the cell interface \( \Sigma_p \).

The numerical flux in \( x \)-direction is given as an example
\begin{equation}
    F_p(t) = \sum_{m,n=1}^{3} \omega_{mn} \int \psi u f(x_{i+1/2,jm,kn}, t, u, \xi) d\xi \Delta y \Delta z.
\end{equation}

The Gaussian quadrature is used over the cell interface, where \( \omega_{mn} \) is the quadrature weight, \( x_{i+1/2,jm,kn} = (x_{i+1/2}, y_{jm}, z_{kn}) \) and \( (y_{jm}, z_{kn}) \) is the Gauss quadrature point of cell interface \( y_j \times z_k \). The gas distribution function \( f(x_{i+1/2,jm,kn}, t, u, \xi) \) in the local coordinate can be given by the integral solution of Eq.(1) as
\begin{equation}
    f(x_{i+1/2,jm,kn}, t, u, \xi) = \frac{1}{\tau} \int_0^t \int_0^\xi g(x', t', u, \xi') e^{-\eta(t'-\xi')/\tau} d\eta' + e^{-\eta/\tau} f_0(-u, \xi),
\end{equation}
where \( x' = x_{i+1/2,jm,kn} - u(t - t') \) is the trajectory of particles, \( f_0 \) is the initial gas distribution function, and \( g \) is the corresponding equilibrium state. In GKS framework, the second-order gas distribution function at cell interface has been constructed\textsuperscript{11}. After the gas distribution function being determined, the numerical flux can be obtained by taking moments of it as Eq.(5). To achieve high-order accuracy in space and time, the high-order spatial reconstruction and the multi-stage time discretization has been systematically developed in Refs\textsuperscript{3,14}. In current study, the well-developed fourth-order three-dimensional (3D) parallel HGKS code will be used to provide the high-accuracy flow-fields for iLES and eLES. For turbulence simulation, more details in fourth-order HGKS can be found in Ref\textsuperscript{17}.

When implementing the eLES models, an extended BGK equation has been proposed as
\begin{equation}
    f_i + u f_i + v f_j + w f_z = \frac{g-f}{\tau + \tau_i},
\end{equation}
where \( \tau_i \) is an enlarged turbulent relaxation time. Based on the Chapman-Enskog expansion, Eq.(7) can recover the eddy viscosity model according to the following relation between turbulent eddy viscosity \( \mu_t \) and turbulent relaxation time \( \tau_i \) as
\begin{equation}
    \tau + \tau_i = \frac{\mu + \mu_t}{p},
\end{equation}
where static Smagorinsky model (S-model)\textsuperscript{1} and Vreman-type model (V-model)\textsuperscript{3} are used to obtain the turbulent eddy viscosity \( \mu_t \) in Eq.(8). The detailed implementations and comparisons among different eddy viscosity models within the HGKS framework has been conducted in Ref\textsuperscript{11}. In following study, the S-model is equipped with the coefficient \( C_\tau = 0.1 \), and V-model adopts corresponding coefficient as \( C_v = 2.5C_s^2 = 0.025 \).

III. RESULTS AND ANALYSIS

In this section, iLES and eLES are implemented in compressible Taylor-Green vortex problem (TGV). Priori coarse-grained analysis of DNS solution sheds light on expected modeling SGS dissipation, and the quantitative SGS dissipation analysis will be presented subsequently.

A. Numerical Simulation in TGV

Taylor-Green vortex is a classical problem in fluid dynamics developed to study vortex dynamics, turbulent transition, turbulent decay and energy dissipation process\textsuperscript{22,23}. The flow is computed within a periodic square box defined as \( -\pi L \leq x, y, z \leq \pi L \). Fluid is a perfect gas with \( \gamma = 1.4 \) and Prandtl number \( Pr = 1 \). Mach number takes \( Ma = 0.1 \) and Reynolds number is \( Re = 1600 \). The detailed set-up can be found in Ref\textsuperscript{17}. In current simulation, iLES and eLES are simulated in 256\textsuperscript{3} grids.

To evaluate the performance of iLES and eLES, several diagnostic dynamic quantities are computed. The ensemble (volume-averaged) turbulent kinetic energy \( E_k \) is
\begin{equation}
    E_k = \frac{1}{\rho_0 \Omega} \int \frac{1}{2} \rho U_i U_i d\Omega,
\end{equation}

where \( \rho_0 \) is the initial density, \( \Omega \) the volume of whole computational domain, \( \cdot \) the inner product. The ensemble enstrophy dissipation rate \( \varepsilon(\zeta) \) is related to the enstrophy \( \zeta \) as

\[
\varepsilon(\zeta) = \frac{2\mu}{\rho_0} \zeta,
\]

\[
\zeta = \frac{1}{\rho_0 \Omega} \int \frac{1}{2} \rho \omega_k \cdot \omega_k \, d\Omega,
\]

where vorticity is \( \omega_k = \epsilon_{ijk} U_{ik,j} \) with \( \epsilon_{ijk} \) the alternating tensor and \( U_{k,j} = \partial U_i / \partial x_j \). \( \varepsilon(\zeta) \) is utilized to evaluate the resolution of resolved turbulent structures. For the compressible flow, the ensemble physical dissipation rate \( \varepsilon_{phy} \) obtained from the NSE is the sum of three contributions

\[
\varepsilon_{phy} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3,
\]

\[
\varepsilon_1 = \frac{2\mu}{\rho_0 \Omega} \int S^+_{ij} \cdot S^+_{ij} \, d\Omega, \\
\varepsilon_2 = \frac{\mu_b}{\rho_0 \Omega} \int \theta^2 \, d\Omega, \\
\varepsilon_3 = -\frac{1}{\rho_0 \Omega} \int \rho \theta \, d\Omega,
\]

where \( S^+_{ij} \) is the deviatoric part of the strain rate tensor \( S_{ij} \), with \( S^+_{ij} = S^*_{ij} - \delta_{ij} S_{kk}/3, S_{ij} = (U_{ij} + U_{ji})/2 \). \( \cdot \) denotes the product for second-order tensor. \( \mu_b \) is the bulk viscosity, and the inherent bulk viscosity is \( \mu_b = 4\mu / 15 \) for BOK model. \( \theta = U_{i,j} \) denotes the divergence of turbulent velocity. To eliminate the post-processing error from numerical discretization, all spatial derivatives in Eq.(10) and Eq.(11) are computed by sixth-order central difference.

Figure 1 presents the time history of ensemble turbulent kinetic energy \( E_k \). Compared with the DNS solution, we observe that the first-order statistical variable \( E_k \) is not sensitive to the grid resolution, as well as iLES or eLES models. Figure 2 clearly presents that iLES performs better than eLES, entailing iLES resolve much accurate turbulent structures. In current compressible simulation with small Mach number \( Ma = 0.1 \), Figure 3 shows that primary dissipation rate \( \varepsilon_1 \) is the dominant contribution to ensemble physical dissipation rate \( \varepsilon_{phy} \). Meanwhile, dominant ensemble dissipation rate \( \varepsilon_1 \) in Figure 3 again to show that iLES outweighs eLES on the exactly same unresolved grids. The similar conclusion has been drawn in previous simulation of compressible separated turbulent flow, where iLES outweighs eLES in compressible turbulent flow over periodic hills. In terms of ignorable ensemble dissipate rate \( \varepsilon_2 \) and \( \varepsilon_3 \), iLES and eLES are in the quite similar performance.

**B. Priori Analysis of \( K_{sgs}^f \)**

To study the seemingly abnormal performance of iLES and eLES, we firstly focus on the priori coarse-grained analysis of filtered SGS turbulent kinetic energy \( K_{sgs}^f \) to evaluate the filtered SGS production of \( K_{sgs}^f \) quantitatively. The following DNS flow-fields have been obtained as case \( \Gamma G_3 \) in Ref, 17, 19, 25, 27.

\[
\langle \overline{\rho K_{sgs}^f} \rangle_{ij} + \langle \overline{\rho K_{sgs}^f \overline{U}_j^f} \rangle_{ij} = P_{sgs}^f - D_{sgs}^f + \Pi_{sgs}^f + T_{sgs}^f,
\]

where \( \overline{\cdot} \) denotes the time average.

FIG. 1. Time history of ensemble turbulent kinetic energy \( E_k \). The DNS solution with 1024 grids is provided in Ref. 17.

FIG. 2. Time history of ensemble enstrophy dissipation rate \( \varepsilon(\zeta) \).
where $P_{\text{SGS}}^{f}$ is the filtered SGS production term, $D_{\text{SGS}}^{f}$ the filtered SGS dissipation term, $\Pi_{\text{SGS}}^{f}$ the filtered SGS pressure dilation term, and the last term $T_{\text{SGS}}^{f}$ the sum of filtered SGS diffusion terms. The detailed right-hand-side terms in Eq. (12) can be found in Ref. 16. Be of scientific interest, we pay special attention to the filtered SGS production term as

$$P_{\text{SGS}}^{f} = -\tau_{ij}^{f} S_{ij}^{f},$$

(13)

with filtered $S_{ij}^{f} = 1/2(\tilde{U}_{ij}^{f} + \tilde{U}_{ji}^{f})$. It is well known that filtered SGS production term $-\tau_{ij}^{f} S_{ij}^{f}$ represents the inter-scale transfer associated with the interaction of the resolved and unresolved scales.  

Figure 4 qualitatively presents the contours of filtered SGS turbulent kinetic energy $K_{\text{SGS}}^{f}$. It is observed that $K_{\text{SGS}}^{f}$ is time-dependent during the unsteady evolution process. Contours of forward and backward filtered SGS turbulent energy transfer are presented in Figure 5 and Figure 6. Forward and backward filtered SGS turbulent energy transfer is clearly observed. Filtered SGS turbulent kinetic energy backscatter illustrates the SGS turbulent kinetic energy transfer from subgrid scales to resolved scales. Unfortunately, we know that backward energy transfer cannot be modeled by both iLES and eLES with static coefficients.

Table 1 quantitatively presents that $E_{k}$ is in the order of $O(10^{4})$ to $O(10^{2})$ of the $\langle K_{\text{SGS}}^{f} \rangle$ during the evolution process. Dominant physical dissipate rate $\epsilon_{1}$ is approximately 20 times larger than the ensemble filtered SGS production rate $\langle -\tau_{ij}^{f} S_{ij}^{f} \rangle$. When constructing eLES models, the modeling SGS dissipation of eLES models is expected to be pointwise equivalent to the filtered SGS production term $-\tau_{ij}^{f} S_{ij}^{f}$. As presented in Table 1, the ensemble filtered SGS production term is far smaller than the dominant ensemble physical dissipation. We know eLES always provides the positive modeling
SGS dissipation without considering the numerical dissipation. However, in practical simulation, the built-in numerical dissipation always get involved with the process of total SGS dissipation. On unresolved grids, the magnitude of built-in numerical dissipation rate may be larger than the filtered SGS production rate $-\tau_{ij}^f \tilde{S}_{ij}$, thus the explicit modeling SGS dissipation is not required under such circumstance. Up to this point, we have limited our discussion in priori analysis, and the posteriori performances will be evaluated thereafter.

Before trusting eLES models without thinking, above priori analysis has reminded us to evaluate the built-in numerical dissipation quantitatively. We follow the procedures for iLES analysis in incompressible LES\(^9\). For compressible LES, without considering the numerical discrete error, the momentum equation reads

$$\frac{\partial \rho \tilde{U}_i}{\partial t} + \frac{\partial \rho \tilde{U}_i \tilde{U}_j}{\partial x_j} = -\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}^f}{\partial x_j}, \quad (14)$$

with SGS stress $\tau_{ij} = \overline{\rho (U_i \tilde{U}_j - \tilde{U}_i \tilde{U}_j)}$, and $\sigma_{ij} = 2\mu \tilde{S}_{ij}$ with $\tilde{S}_{ij}$ defined as Eq.(11). Conceptually, we can define the discrete derivative operator as $\delta^s_i$ the temporal discrete derivative operator, and $\delta^s_{ij}$ the spatial discrete derivative operator. Considering the numerical discrete error, the modified equation (numerical resolved equation) of Eq.(14) reads

$$\frac{\delta^s \rho \tilde{U}_i}{\delta^s t} + \frac{\delta^s \rho \tilde{U}_i \tilde{U}_j}{\delta^s x_j} = -\frac{\delta^s \tau_{ij}}{\delta^s x_j} - \frac{\delta^s \tau_{ij}^f}{\delta^s x_j} - \frac{\delta^s \tau_{ij}^{num}}{\delta^s x_j}, \quad (15)$$

where $\tau_{ij}^{num}$ is the explicit modeling SGS stress in well-developed eLES\(^2-5\), while all numerical discrete errors are effectively grouped into $\tau_{ij}^{num}$ phenomenologically. Numerical discrete error is very hard to analyze term by term in finite-volume framework, since the errors result from the spatial reconstruction procedure, time discretization procedure, the design of flux, and the averaging process when updating conservative variables. The numerical error is grid resolution-dependent, numerical scheme-dependent and turbulence type-dependent, thus determining its quantitative expression seems extremely difficult.

In view of this dilemma, we adopt to deal with the total SGS dissipation, which is a classical route to understand the eLES models in LES community. In practical simulations, corresponding to Eq.(15), the pointwise total SGS dissipation rate $\varepsilon_{sgs}^p$ contains two parts

$$\varepsilon_{sgs}^p = \varepsilon_{sgs}^{mod} + \varepsilon_{sgs}^{num},$$

$$\varepsilon_{sgs}^{mod} = -\tau_{ij}^f \tilde{S}_{ij},$$

$$\varepsilon_{sgs}^{num} = -\tau_{ij}^{num} \tilde{S}_{ij},$$  \quad (16)

### TABLE I. Ensemble turbulent kinetic energy $E_k$, ensemble filtered SGS turbulent kinetic energy $\langle K_{sgs}^f \rangle$, ensemble dominant dissipation rate $\varepsilon_1$ and ensemble filtered SGS production term $\langle -\tau_{ij}^f \tilde{S}_{ij}^f \rangle$ at $t = 2.5, 5, 10$ and 15. $E_k$ and $\varepsilon_1$ are obtained from case $TG_3$ in Ref\(^{17}\).

<table>
<thead>
<tr>
<th>Time</th>
<th>$E_k$</th>
<th>$\langle K_{sgs}^f \rangle$</th>
<th>$\varepsilon_1$</th>
<th>$\langle -\tau_{ij}^f \tilde{S}_{ij}^f \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>0.123</td>
<td>$2.6 \times 10^{-9}$</td>
<td>$8.8 \times 10^{-9}$</td>
<td>$1.3 \times 10^{-9}$</td>
</tr>
<tr>
<td>5</td>
<td>0.118</td>
<td>$1.2 \times 10^{-9}$</td>
<td>$4.1 \times 10^{-9}$</td>
<td>$1.3 \times 10^{-9}$</td>
</tr>
<tr>
<td>10</td>
<td>0.074</td>
<td>$3.3 \times 10^{-9}$</td>
<td>$1.1 \times 10^{-9}$</td>
<td>$5.1 \times 10^{-9}$</td>
</tr>
<tr>
<td>15</td>
<td>0.036</td>
<td>$1.3 \times 10^{-9}$</td>
<td>$4.5 \times 10^{-9}$</td>
<td>$1.3 \times 10^{-9}$</td>
</tr>
</tbody>
</table>
Eq.(16) shows that the total SGS dissipative behavior is determined by both explicit modeling SGS dissipation rate \( \varepsilon_{\text{mod}} \) and built-in numerical SGS dissipation rate \( \varepsilon_{\text{num}} \). We notice that there is no explicit modeling SGS dissipation in iLES. While, the built-in numerical dissipation is usually ignored in eLES. In terms of the free decaying TGV, ensemble total dissipation rate \( \varepsilon(E_k) \) of turbulent kinetic energy and ensemble total SGS dissipation rate \( \varepsilon_{\text{sgs}} \) can be computed by

\[
\varepsilon(E_k) = -\frac{dE_k}{dt},
\]

\[
\varepsilon_{\text{sgs}} \equiv \langle \varepsilon_{\text{sgs}}^\rho \rangle = \varepsilon(E_k) - \varepsilon_{\text{phy}},
\]

with second-order central difference method in computing \( \varepsilon(E_k) \). Again, the discrete error in post-processing procedure is assumed to be neglected. \( \varepsilon_{\text{phy}} \) denotes the ensemble resolved physical dissipation rate as Eq.(11).

![Image](image_url)

**FIG. 7.** Time history of ensemble total dissipation rate \( \varepsilon(E_k) \).

<table>
<thead>
<tr>
<th>Time</th>
<th>iLES</th>
<th>S-Model</th>
<th>V-Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>( 1.5 \times 10^{-5} )</td>
<td>( 2.8 \times 10^{-5} )</td>
<td>( 2.6 \times 10^{-5} )</td>
</tr>
<tr>
<td>5</td>
<td>( 1.4 \times 10^{-4} )</td>
<td>( 3.5 \times 10^{-4} )</td>
<td>( 3.2 \times 10^{-4} )</td>
</tr>
<tr>
<td>10</td>
<td>( 6.7 \times 10^{-4} )</td>
<td>( 1.4 \times 10^{-3} )</td>
<td>( 1.3 \times 10^{-3} )</td>
</tr>
<tr>
<td>15</td>
<td>( 1.8 \times 10^{-3} )</td>
<td>( 2.5 \times 10^{-3} )</td>
<td>( 1.8 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

**TABLE II.** Ensemble total SGS dissipation rate \( \varepsilon_{\text{sgs}} \) with iLES and eLES at \( t = 2.5, 5, 10 \) and 15.

![Image](image_url)

**FIG. 8.** Time history of ensemble total SGS dissipation rate \( \varepsilon_{\text{sgs}} \).

on eLES is approximate 2 times larger than that of iLES, because the static eddy viscosity model always provides the positive modeling SGS dissipation. Additionally, we observe that the posteriori ensemble total SGS dissipation rate \( \varepsilon_{\text{sgs}} \) in Table II is larger than the priori ensemble filtered SGS production term \( \langle -\tau_{ijj}^\rho S_{ijj} \rangle \) in Table I, except for the late decaying stage at \( t = 15 \). We revisit the time history of ensemble enstrophy dissipation rate \( \varepsilon(\zeta) \) in Figure 2. It can be concluded that the additional explicit models in eLES pollutes the resolved turbulent structures, i.e., blurs the resolution of resolved vorticity. To strengthen above conclusion, effects of static eddy viscosity models on density, momentum and energy transport will be explored, beyond grouping the explicit modeling effects into the effective ensemble modeling SGS dissipation.

IV. CONCLUSION AND DISCUSSION

To address the better performance of iLES, current research conducts the quantitative comparisons between iLES and eLES, especially focusing on the built-in numerical dissipation and explicit modeling SGS dissipation. It is concluded that the numerical dissipation in iLES can act as the intrinsic SGS dissipation, and explicit modeling SGS dissipation is not required in low-Reynolds number turbulence. In addition, the additional explicit SGS models in eLES even pollute the resolved turbulent structures. An important consequence is that the improvement of the reliability of LES results requires work on both the numerical methods and the subgrid models. In following studies, more detailed analysis in Eq.(15) deserves to be explored. iLES for complex turbulent flows is still under debate, current quantitative analysis of total SGS dissipation gives the specific hints on this issue. More importantly, the LES community should pay special attention to the utilization of static explicit eddy viscosity models, instead of regarding the eLES as holy grail in LES on unresolved grids.
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