Characterizing discretization and filter effects on LES via DNS-assisted evaluations

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The current investigation looks at the effect of discretization and filtering schemes on LES numerical errors. Specifically, the impact of low- versus high-order central differencing stencils is judged relative to employing non-unity filter-to-grid ratios via explicit filtering; in addition, the use of smooth versus scale-discriminant filter formulations is considered. A quasi *a-priori* approach that utilizes data from a tandem DNS calculation is used to perfectly close the LES equations and evolve the set of filtered governing equations on the coarser LES grid. As a result, modeling errors are avoided and the role of the numerical treatment (i.e., discretization and the LES filter) is isolated. The quasi *a-priori* technique is applied to the full reactive Navier-Stokes system, for which a premixed flame test case is considered, thus providing evaluations of the schemes in the presence of sharp gradients.

1. Introduction

The design and optimization of reactive flow engineering systems requires the ability to leverage predictive computational fluid dynamics. Large-eddy simulation (LES) presents itself as a viable candidate for such computations owing to its ability to represent transient dynamics without resolving all the length scales in the flow. The success of the LES methodology as a predictive tool depends on the development of accurate, physics-based models responsible for representing the effect of subfilter dynamics on resolved modes. Specific to reacting flows, this includes important phenomena such as flame-turbulence interaction and energy backscatter (Poludnenko & Oran 2010; Towery et al. 2016).

Reducing the role of discretization error is imperative in isolating the true characterization of model performance, for the former can interact with the latter and impact the solution (Klein et al. 2008). For example, Cocks et al. (2015) compare several codes and observe that the results for the reacting flow cases do not agree, whereas the non-reacting flow solutions are consistent across codes. Each implementation uses the same closure model and identical grids; therefore, the disagreement in the results highlights an increased sensitivity to either the numerical schemes or the interactions of the numerical schemes with the combustion closure model. Understanding how best to separate the numerics and model, as well as how to mitigate the influence of numerics once separated, thus becomes crucial for the assessment and development of LES models.

When direct numerical simulation (DNS) calculations are feasible, one can employ *a-priori* analysis techniques to understand how LES parameters, such as filter shape and filter width, can affect model accuracy. Unfortunately, this approach neglects the

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The quasi \textit{a-priori} approach has previously been used in nonreacting flows to study various topics such as sensitivity of the filter shape to closure errors (DeStefano & Vasilyev 2002) and the performance of different models relative to explicit and implicit filtering (DeStefano & Vasilyev 2004; Li & Wang 2016). In the context of reacting flows, Edwards & Nielsen (2018) study various mesh-sequence realizations and employ the finest grid to provide reaction rate closure models for the coarser grids. Kaul & Raman (2011) use a similar closure approach to investigate discretization errors relative to scalar variance modeling.

The current study focuses on the choice of discretization schemes relative to the LES formulation (e.g., filter type, filter width) and its effects on overall solution accuracy when compared with reference data (i.e., filtered DNS). Specifically, focus is placed on the potential benefits associated with employing non-unity filter-to-grid ratios (FGR) via explicit filtering and the relative impact of high-order discretizations and scale-discriminant filters. This is done with the goal of discerning best practices in the formulation of an LES calculation in order to mitigate the impact of numerical error. Such understanding would be beneficial for both informing \textit{a-posteriori} calculations and setting up a proper testbed without discretization errors, useful for model evaluations. The above topics are thus explored via a quasi \textit{a-priori} approach that closes all equations of the reactive Navier-Stokes system with a perfect model, recovering the filtered equations. The current study considers a triply periodic turbulent premixed flame configuration that is DNS accessible, for which the various computations have been carried out primarily between two different codes, LESLIE (Georgia Institute of Technology) and CASTLES (Air Force Research Laboratory).

Section 2 details the current quasi \textit{a-priori} approach and describes the numerical infrastructures employed. Specifics of the turbulent premixed test case along with initial DNS characterizations are introduced in Section 3. LES results demonstrating the effect of discretization scheme, filter type and filter width are then presented from various perspectives (e.g., $L_2$ error, energy spectra, statistics). Initial conclusions and directions for future work are given in Section 4.

2. The quasi \textit{a-priori} approach

The quasi \textit{a-priori} approach solves the LES equations (written here in a general residual form),

\[ d_t \hat{Q} | \text{LES} = R(\hat{Q}) | \text{LES} + T(Q) \quad \text{with} \quad T(Q) = \hat{R}(Q) | \text{DNS} - R(\hat{Q}). \] (2.1)
The closure term $T(Q)$ is then supplied in a time-accurate fashion from a DNS calculation. The current implementation features a parent DNS calculation that is ran in tandem with several children LES runs. Closure information is exchanged at each stage of the temporal integration procedure. The time step size, temporal integration scheme, and boundary conditions are the same for the parent DNS and all children LES simulations (note that the LES is initialized with the Favre-filtered DNS initial conditions). However, each of the LES calculations can support a different grid resolution, spatial discretization scheme, or explicit filter size and shape. In this way, a large parameter space of LES configurations may be explored efficiently.

DeStefano & Vasilyev (2002) first introduce the quasi a-priori idea and employ a closure of the form: $T(Q) = \hat{R}(Q)|_{DNS} - \hat{R}(Q)|_{LES}$. For example, with respect to the nonlinearity found in the one-dimensional Burgers equation, this corresponds to $T = (u^2_{DNS} - \hat{u}^2_{DNS})/2$. DeStefano and Vasilyev thus build the exact functional form of the closure from the filtered DNS data. In the current study, a different interpretation is used and $T(Q) = \hat{R}(Q)|_{DNS} - \hat{R}(Q)|_{LES}$ is chosen. Substitution into Eq. (2.1) above perfectly recovers the filtered-DNS equations,

$$d_t \hat{Q}_{|LES} = \hat{R}(Q)|_{DNS} \quad \text{with} \quad R(Q) = \delta_{x_j} F_j(Q) + S(Q),$$

where the vector $F_j(Q)$ represents fluxes in direction $j$ to be discretely differentiated by the operator $\delta_{x_j}$ on the LES grid, while $S(Q)$ represents source terms (e.g., reaction terms). On the other hand, note that substituting the original closure employed by DeStefano and Vasilyev would append a corrective drift-like term $D = \hat{R}(Q)|_{LES} - \hat{R}(Q)|_{DNS}$ to Eq. (2.2). By neglecting this drift term, the solution is evolved without any feedback mechanism for $\hat{Q}_{|LES}$. Consequently, one should expected errors to accumulate monotonically in time, representing a steady divergence between the reference and LES solutions. Nevertheless, the closure approach presently considered will highlight numerical errors due to discretization on the LES grid and furthermore avoids potential realizability issues relating to evaluating thermodynamic and reactive terms in the residual.

The transfer of information from the parent DNS grid to the child LES grid is represented in terms of the filter operation $(\hat{\cdot})$. However, it is important to distinguish the filtering-like effect of projecting onto a coarser grid via $(\hat{\cdot})$ from explicitly filtering the data once on the coarse grid $(\hat{\cdot})$ (Carati et al. 2001). One can define the overall filter as a combination of these actions such that $(\hat{\cdot}) = (\hat{\cdot})$. In the case of implicit or grid filtering, one has $(\hat{\cdot}) = (\hat{\cdot})$. In the case of explicit filtering, one can recover $(\hat{\cdot}) \approx (\hat{\cdot})$, with the approximation becoming more accurate as the FGR increases.

The current investigations were carried with two different codes (LESLIE and CASTLES) in order to help cross-validate observed trends and conclusions. However, for the sake of brevity, the results presented herein are exclusively from CASTLES (the Cartesian portion of the SPACE platform (Harvazinski et al. 2018), which employs central finite-differencing (CD) of various orders and integrates in time using a third-order Runge-Kutta method. The compressible reactive Navier-Stokes system is solved with a conservative form of $F_j$. Furthermore, the current calculations employ uniform Cartesian meshes wherein coarser grids are collocated within the DNS grid (see Figure 1).

The CASTLES code uses implicit (i.e., Padé) discrete Tangent stencils (Raymond & Garder 1991) for its explicit filtering. The second-order Tangent (Tan02) filter constitutes an averaging operator (all weights positive) in physical space for FGR $\geq 2$ and is thus monotone preserving, similar to the top-hat (TH) filter kernels traditionally applied in
Figure 1. Depiction of DNS parent data being projected from a fine Cartesian grid onto collocated LES child grids via a filtering procedure (e.g., top-hat, spectral sharp).

Figure 2. Damping response functions at different FGR for (a) a top-hat filter (TH), (b) a second-order Tangent filter (Tan02) such that $|G|((k\Delta) = 0.5$ and (c) a sixth-order Tangent filter (Tan06) such that $|G|((k\Delta) = 0.5$.

LES. The sixth-order Tangent (Tan06) filter, on the other hand, may not have all positive weights and therefore can admit new overshoots or undershoots in a filtered signal; this may cause issues in the presence of shocks or sharp gradients and may offset the benefits of having a sharper filter in spectral space. The respective damping responses of the filters are plotted in Figure 2 for various FGR. Note that the top-hat has its filter width defined in physical space (i.e., $\Delta = r\Delta x$) while the Tangent filters define the filter width in terms of the spectral response such that $|G|((k\Delta) = 0.5$. Increasing the FGR generally attenuates a larger portion of the small scales while reducing the range of scales resolved by the LES calculation. The delicate balance between removing error at the small scales and losing usable information is one of the aspects that makes the choice between explicitly filtered and implicitly filtered LES nontrivial (Lund 2003).

With respect to projecting information from the DNS grid to the LES grid, different procedures may be employed. In the case of CASTLES, a physical comb filter, or full-weighting, is chosen for the projection procedure. This results in a subsampling of the DNS data, which could potentially introduce aliasing artifacts. The full-weighting is required here, however, because the CASTLES code evolves the primitive variables such
that \( d_t Q_{prim} = \Gamma^{-1} R_{cons} = \Gamma^{-1} [\delta_x F_j + S] \). In the context of evaluating the residual on the LES grid, one would need to satisfy \( \Gamma^{-1} R_{cons} = \Gamma^{-1,*} R_{cons} \), where the new Jacobian \( \Gamma^{-1,*} \) incorporates subgrid closure information. Subsampling via full-weighting should thus avoid this complexity by rendering the filtering to be point-wise (rather than spatially coupled) and thus allowing \( \Gamma^{-1} = \Gamma^{-1,*} \) (i.e., the Jacobian is evaluated directly at the subsampled points).

### 3. Computational results

#### 3.1. Test case overview

Initial conditions for the current test case were provided by Qing Wang and Matthias Ihme of the Center for Turbulence Research (private communication). The initial flow field consists of a spherical region of premixed methane-air reactants surrounded by the adiabatic flame products. This is overlaid upon a field of turbulent velocities that is initialized via a von Kármán-Pao (vKP) energy spectrum (Pope 2000). The flame is derived from a one-dimensional laminar flame calculated at a unity equivalence ratio \( (\phi = 1) \), yielding a flame speed of \( S_F = 0.40 \ [m/s] \) and a flame thickness of \( \delta_F = 4.2 \times 10^{-4} \ [m] \). The initial radius of reactants is \( 3 \ [mm] \) and the calculation is carried out in a \( L^3 = 10 \times 10 \times 10 \ [mm^3] \) periodic box. Turbulence, chemical, and numerical characterizations relative to the initial condition are summarized in Table 1. Placement with respect to a regime diagram would indicate the current problem to be within the thin reaction zone regime, near the border of the broken reaction zone regime. A two-step chemical mechanism for the methane-air reaction is used,

\[
CH_4 + 1.5O_2 \rightarrow CO + 2H_2O ,
\]

\[
CO + 0.5O_2 \rightarrow CO_2 .
\]  

The reaction rates for the mechanism can be found in Wang & Ihme (2017). All calculations are carried out with a well-resolved time step size of \( \Delta t = 10^{-8} \ [s] \). Owing to the decaying nature of the problem, the following results will consider \( t = 4.0 \times 10^{-4} \ [s] \) where the turbulence is still active and the reactants have not been entirely consumed. Figure 3 shows the temperature field at the initial condition on the \( N = 256^3 \) DNS grid and then at the principal evaluation time of \( t = 4.0 \times 10^{-4} \ [s] \).

#### 3.2. LES results

The following section explores the effect of filter-to-grid ratio (FGR) relative to the numerical discretization and filter type. Conclusions between the two codes were found to be consistent; therefore, the following results are from the CASTLES code for brevity.

Figures 4(a–c) depict various instantaneously filtered DNS (IF-DNS) temperature

<table>
<thead>
<tr>
<th>( Re_t )</th>
<th>( Ka )</th>
<th>( S_F \ [m/s] )</th>
<th>( \delta_F \ [m] )</th>
<th>( \Delta t \ [s] )</th>
<th>( \Delta x \ [m] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>364</td>
<td>0.40</td>
<td>( 4.2 \times 10^{-4} )</td>
<td>( 10^{-8} \sim 10^{-4} \tau_\eta )</td>
<td>( 0.01 \frac{\eta_0}{256} \sim 1.7 \eta \sim 0.10 \delta_F )</td>
</tr>
</tbody>
</table>

Table 1. Summary of parameters for initial condition of turbulent premixed flame relative to the \( N = 256^3 \) grid.
Figure 3. Solution slices of the center Z-plane temperature at (a) the initial condition and (b) at the principal evaluation time $t = 4.0 \times 10^{-4} \ [s]$ on the $N = 256^3$ DNS grid.

Figure 4. Temperature slices of the center Z-plane at the principal evaluation time $t = 4.0 \times 10^{-4} \ [s]$ on the $N = 64^3$ child grids with the Tan02 filter for (a) IF-DNS at FGR = 1, (b) IF-DNS at FGR = 2, (c) IF-DNS at FGR = 4, (d) QPriori at FGR = 1, (e) QPriori at FGR = 2 and (f) QPriori at FGR = 4.

Figure 5 presents the $L_2$ relative errors of temperature as a function of the spatial discretization order for the convective or transport terms, showing second- through eighth-order central differencing (CD02, CD04, CD06, CD08). Note that diffusion terms are kept to second order. In all cases, the error is seen to increase monotonically and linearly...
in time after an initial rapid increase. This is a consequence of the QPriori right-hand side being passive (i.e., having no feedback mechanism relative to the solution variable, $\hat{Q}_{LES}$), so the solution steadily accumulates the differencing error. However, we note that increasing the FGR reduces the error magnitude consistently. Furthermore, the amount of error changes on the basis of discretization order. For a unity FGR (i.e., implicit or grid filtering), the fourth- through eighth-order schemes outperform the second-order method but are nearly indistinguishable from each other. Increasing the FGR shows slightly more differences between the schemes; however, employing a fourth-order discretization seems to be sufficient in general. This demonstrates the competing effects of admitting small scales that may be polluted with numerical error versus reducing the range of resolved wavenumbers and retaining accuracy. At a small FGR, the solution may be dominated by the inability to calculate small-scale features, thus producing noise or Gibbs phenomenon; however, when focusing on the larger scales (which are more accurately calculated), one then notices the benefits of the higher-accuracy schemes.

One can also consider how the type of filter affects error characteristics. Figure 6 compares the Tan02 and Tan06 filters for the CD02 and CD08 discretizations at various
Figure 7. Turbulent kinetic energy spectra at $t = 4.0 \times 10^{-4}$ [s]. IF-DNS and QPriori runs on $N = 64^3$ grids for (a) FGR = 1 and (b) FGR = 4 (Tan02 filter) are compared.

Figure 8. Temperature PDFs at $t = 4.0 \times 10^{-4}$ [s] on a $N = 64^3$ grid for (a) the instantaneous filtered DNS reference solution at FGR = 1 and for quasi *a-priori* LES with CD02 at (b) FGR = 1 and (c) FGR = 2 with Tan02.

FGR. In all instances except for the CD02 scheme at FGR = 8, the Tan06 filter shows more relative error than the Tan02 variant (note that the IF-DNS and the LES use the same filter). This is likely tied to the fact that the spectrally sharper Tan06 filter is not monotone preserving and thus could amplify numerical oscillations already generated by the central differencing scheme. This presents a challenge in terms of how to employ scale-discriminant filters on complex topologies and suggests the need for proper spatial adaptivity of such filters.

Next, Figure 7 presents the kinetic energy spectra characterization in terms of integral wavenumber magnitude (note that binning has been performed) for the CD02 and CD08 schemes. In the case of implicit filtering (i.e., FGR = 1) shown in Figure 8(a), the LES calculations have acquired a large amount of energy in the high wavenumbers, corresponding to small-scale noise. On the other hand, Figure 8(b) shows that employing explicit filtering with FGR = 4 allows the LES to better match the IF-DNS.

Finally, inspecting the statistics is also insightful in characterizing the impact of the discretization and the filter. Temperature probability distribution functions (PDFs) are presented in Figure 8. Here, the benchmark distribution is taken to be the under-sampled DNS on the $N = 64^3$ grid (i.e., FGR = 1). The second-order LES without explicit filtering is then seen to have a slightly larger variance—a consequence of generating new extrema in the distribution (in this case leading to some unrealizable values). Meanwhile,
employing monotonic explicit filtering at $FGR = 2$ is seen to decrease the level overshoots and undershoots and reduces the variance of the distribution relative to the nonfiltered result.

4. Conclusions

The current investigation has quantified the performance of central differencing schemes (second- through eighth-order) relative to that of LES parameters such as the type of filter (e.g., second- versus sixth-order implicit Tangent filters) and the FGR. The quasi $a$-priori approach enables one to observe the dynamic influence of numerical error on the LES solution and has been employed for the first time on the full reacting Navier-Stokes system. Summarizing results and observations include: 1) a general reduction in error via high-order discretizations, 2) a further reduction of error by employing increasing FGR by means of explicit filtering and 3) the potential for violations in realizability due to nonmonotone-preserving filters.

Observations regarding the effects of discretization order and FGR on error are consistent with previous theoretical and numerical studies of nonreacting flow settings (Ghosal 1996; Chow & Moin 2003) and support the combined use of high-order methods and non-unity FGR via explicit filtering for effective numerical error mitigation. Although utilizing $FGR > 1$ removes small-scale error, the range of resolved modes is simultaneously decreased. Consequently, employing spectrally sharp LES filters is anticipated to maximally retain the spectral content up to a given scale cutoff. Violation of monotonicity preservation from the use of such spectrally sharp filters, however, is challenging in the presence of sharp gradients (e.g., flame fronts) as new local extrema can lead to nonrealizable thermodynamic values. As a result, the efficient application of explicit filtering to reacting flows requires the development of adaptive stencils for such scale-discriminant filtering schemes and is currently under development.

Future work will look to further apply the quasi $a$-priori technique to confirm the benefits of pairing high-order discretizations with spectral-like filters, first for smooth flow (e.g., Taylor-Green vortex) and then in the presence of sharp gradients, while employing adaptive numerical schemes. Next, the specific performances of explicit filtering techniques such as residual filtering (Gallagher & Sankaran 2018), solution filtering and artificial dissipation (Edoh et al. 2018) in the presence of modeling error will be studied.

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