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Commutator errors in the filtering approach to large-eddy simulation

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We analyze the large-eddy equations that are obtained from the application of a spatially nonuniform filter to the Navier–Stokes equations. Next to the well-known turbulent stress tensor a second group of subgrid terms arises; the so-called commutator errors. These additional subgrid terms emerge in the large-eddy equations solely as a consequence of the nonuniformity of the filter. We compare the magnitude of the divergence of the turbulent stress tensor with that of the commutator errors and pay attention to the role of the explicit filter that is adopted. It is shown that the turbulent stress contributions and the commutator errors display the same scaling behavior on the filter width and its derivative. Correspondingly, the use of higher-order filters is shown not only to decrease the commutator errors but likewise the turbulent stresses are uniformly reduced with increasing filter order. In addition, we establish that skewness of the spatial filter has a strong influence on the magnitude of the commutator errors while leaving the turbulent stress contributions roughly unaltered. The analysis of the order of magnitude of the various terms provides an impression of the flow conditions and filter width nonuniformities which necessitate explicit commutator-error modeling next to the more traditional turbulent stress subgrid modeling. Some explicit models for the commutator errors are put forward and an *a priori* assessment of these commutator-error models in turbulent mixing layers is obtained. Generalized similarity models appear promising in this respect and display high correlation with the exact commutator errors. © 2005 American Institute of Physics. [DOI: 10.1063/1.1852579]

I. INTRODUCTION

The development of accurate simulation strategies for turbulent flows is a topic of intensive ongoing research.¹ The various existing simulation approaches incorporate the intricate details of turbulence to a varying degree. This may be illustrated by distinguishing, e.g., direct numerical simulation (DNS) in which one captures all length scales in a flow, or, large-eddy simulation (LES) in which one explicitly calculates the evolution of the larger scales only while modeling the effect of sufficiently small scales, or, Reynolds averaged Navier–Stokes approaches in which statistical modeling is applied to capture primarily the (steady) mean flow. The amount of retained detail in a simulation is largely governed by the desired accuracy with which a particular flow needs to be represented.

The dynamic complexity of a turbulent flow depends strongly on the Reynolds number Re . In fact, realistic flow conditions correspond to $Re \gg 1$ and typically give rise to flow solutions which are described by a very large number of degrees of freedom. The features in these flows are characterized by a variety of length scales ranging over a number of decades. Turbulent flows at high Re can generally not be captured within the restrictions posed by present-day computational resources using DNS. More importantly, in many applications it is not even required to have explicit access to turbulent flow features of all dynamically relevant length

scales. Therefore, smoothed flow descriptions, such as LES, have been introduced to obtain alternative simulation strategies. LES is aimed at capturing the primary flow features while the dynamical effects of small-scale turbulent contributions are parametrized approximately through the introduction of an explicit subgrid model. This gives rise to a simulation model for turbulent flows that requires only a fraction of the computational effort associated with DNS.

Traditionally, large-eddy simulation was developed within the spatial filtering approach.² In particular, virtually all developments of large-eddy simulation consider spatial filters with constant filter width, e.g., convolution filters.³ In the filtering approach to LES the small scales are effectively removed from the simulation by applying a low-pass filter $\mathcal{L}$, characterized by an externally specified filter width Δ . This suggests the use of a grid with mesh spacing on the order of Δ instead of the Kolmogorov length $\eta \ll \Delta$, in order to obtain a representation of the smoothed LES flow with sufficient numerical accuracy.^{4,5} The filtering allows the computation of the primary flow features at a higher Reynolds number than can be done within a DNS approach. The dynamical effects of the smaller scales are represented by the turbulent stress tensor $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ and have to be modeled in order to close the equations.⁶

The LES approach holds promise to become a relevant

engineering simulation strategy, applicable to flows of realistic complexity, i.e., at high Re, in complex flow domains, involving complicated additional physics related to, e.g., combustion or multiphase flows. However, in order to efficiently extend the LES capabilities to turbulent flows in complex geometries, e.g., including curved and flat walls, displaying regions of separated and reattaching flows, etc., it is required to allow for spatially nonuniform filters $\Delta(\mathbf{x})$.^{7,8} These filters are characterized by a filter width which is an explicit function of spatial coordinates (and possibly also of time⁹). In complex flow domains a lively, small-scale turbulent flow may exist in some parts of the domain while a seemingly laminar flow may simultaneously be present in other parts of the flow domain. The filter width should be reduced, i.e., one locally resolves more scales of the flow, in the “turbulent” parts of the flow domain. Likewise, in regions with comparably quiescent flow the filter width can be chosen larger without notably affecting the accuracy with which the solution is represented. This local refining or coarsening of the description shows some similarity with the use of nonuniform grids in various numerical applications, see, e.g., Ref. 10.

The introduction of a spatially nonuniform filter width complicates the development of the corresponding large-eddy approach since additional closure terms emerge that may or may not require explicit modeling. These terms are generally referred to as commutator-error subgrid terms or simply commutator errors and originate from the fact that nonuniform filtering and differentiation do not commute,^{7,8,11,12} i.e.,

$$\overline{\frac{\partial u}{\partial x}} \neq \frac{\partial \bar{u}}{\partial x}, \quad (1)$$

where the overbar denotes the application of the filter. These commutator errors have been considered before in literature (e.g., Refs. 8, 11, and 13–16), concentrating on their proper definition, the relation with the explicit filter that was used and the role of specialized higher-order filters in connection to the magnitude of these terms. In this paper we extend this work in a number of ways.

A detailed investigation of the commutator errors, their effects on the flow and an estimation of their actual magnitude, using direct numerical simulation data of a turbulent mixing flow, will be considered. This is an essential prerequisite for properly treating these additional closure terms. Especially the scaling of the commutator errors with Δ and its derivatives $\partial\Delta/\partial x_j$ is required before nonuniform filtering with significant gradients in the filter width $\{\|\nabla[\Delta(\mathbf{x})]\| \gg 1\}$ can be applied in actual LES. In this paper we present results of analysis and *a priori* database evaluation. We systematically address two basic questions: (i) under which flow conditions and numerical settings is an explicit modeling of the commutator errors necessary and (ii) what is the quality of specific models proposed to parametrize the commutator errors? We incorporate regular second-order filters, such as the symmetric top-hat and Gaussian filters, as well as high-order filters^{14,15,17} and filters with a skewed support¹⁸ into the investigation. The latter type of filters is sometimes also re-

ferred to as “asymmetric.” However, throughout this paper we will adopt the term “skewed” for these filters.

A first impression of the magnitude and scaling of the commutator errors can be obtained through investigating Taylor expansions of the relevant terms. The present analysis extends earlier work by Ghosal and Moin⁸ who considered symmetric filters. In this paper also skewed filters are considered which significantly alters the findings and introduces dispersion next to dissipation. In LES of flows in complex geometries the use of skewed filters can sometimes be suggested for efficiency reasons or it can be unavoidable, e.g., close to solid walls to circumvent filtering beyond the boundaries, or in regions of rapid spatial variations of turbulence fluctuation levels. The skewness of a filter implies a decrease of the order of the filter which leads to an increase in size of the commutator error.¹⁸ Conversely, an increase in the order of a filter results in a formal decrease of the size of the commutator error and has led to the development of higher-order filters. Higher-order filters have originally been proposed in the context of LES in Ref. 18 and constructed in a specific framework in Refs. 13 and 14. These filters have recently regained interest^{15,19–21} and appear to resolve the issue of explicitly modeling commutator errors in LES. Specifically, the use of a suitable higher-order filter can render the commutator errors arbitrarily small. However, as was shown in Refs. 13 and 18 the use of higher-order filters also leads to a formally equally strong decrease of the contributions of the turbulent subgrid scale flux $\partial_j \tau_{ij}$ in view of the identical dominant scaling behavior with Δ and its derivatives. It is not possible to obtain a separate control over the commutator errors compared to the turbulent subgrid scale fluxes merely by adopting a suitable class of filters. In fact, other measures need to be taken to influence the size of the commutator errors relative to the traditional subgrid terms, as will be indicated in this paper.

The analytical estimates will be complemented by *a priori* evaluations based on DNS data of a turbulent mixing flow.²² This allows to compare the actual magnitude of all commutator-errors and subgrid terms on specific LES grids and for selected filter-width variations. The effect of skewness and of filter order on the subgrid-stress flux (SGS flux) and the commutator errors will be considered. These results establish the actual scaling of the commutator errors and SGS fluxes, confirming the Taylor expansion estimates. The *a priori* comparisons help to globally identify numerical—and flow conditions such that explicit commutator error modeling is required. In particular, if the filter-width variations $\|\nabla[\Delta(\mathbf{x})]\|$ become too large, the commutator errors need to be separately parametrized with appropriate subgrid models. We will propose some explicit commutator-error models and compare their properties with basic properties of the exact commutator errors. Moreover, we will investigate the modeled production and dissipation of turbulent kinetic energy in turbulent mixing layers. The models we will investigate are extensions of similarity—and gradient formulations used previously to model τ_{ij} .^{22–24} *A posteriori* tests of LES with a nonuniform filter width, in which these commutator-error models are considered, will be presented in a forthcoming paper.

The organization of this paper is as follows. In Sec. II the complete nonuniformly filtered Navier–Stokes equations will be introduced. The dependence of the size of the commutator error on the order of the filter will be established in Sec. III and compared with the magnitude of the divergence of the turbulent stress tensor. In Sec. IV results of an *a priori* analysis of the commutator error will be presented. In particular, we will introduce, quantify, and compare several measures for the magnitude of the commutator errors and the SGS fluxes. The *a priori* analysis will focus on effects derived from the order and skewness of the filter. This can be used to identify under which conditions an explicit modeling of the commutator errors is advised. In Sec. V a number of explicit commutator-error models will be introduced and compared with the exact commutator error, focusing on correlation and kinetic energy dynamics. Finally, in Sec. VI we summarize our findings.

II. NONUNIFORM FILTERS AND COMMUTATOR ERRORS

In this section nonuniform filters will be introduced and the application of these filters to the incompressible Navier–Stokes equations will be described. All closure terms arising from nonuniform filtering will be identified and discussed. It will be shown that the filtered velocity field is no longer solenoidal. Moreover, next to the traditional turbulent stress contributions a number of additional closure terms are found which involve the commutator bracket of the filter operator and first- or second-order partial differentiation.

Basic filters for LES can be divided into (closely related) differential—and integral filters.³ In LES these filters are typically low-pass filters, i.e., solutions which vary slowly in space are not affected much by the application of the filter whereas components which are fluctuating more vigorously are effectively reduced by filtering. Here, we will concentrate on integral filters. In one spatial dimension, a general integral filter operator, with nonuniform filter width $\Delta(x)$, can be written as^{14,15}

$$\begin{aligned}\bar{u}(x) &= L(u)(x) = \int_{x_0}^{x_1} g[y-x, \Delta(x)] u(y) dy \\ &= \int_{x_0}^{x_1} \frac{1}{\Delta(x)} G\left(\frac{y-x}{\Delta(x)}\right) u(y) dy,\end{aligned}\quad (2)$$

where x_0 and x_1 denote the boundaries of the flow domain, L is the one-dimensional filter operator mapping of the solution u to the filtered solution $\bar{u}$ and g is referred to as the “total” filter kernel in terms of the “(characteristic) filter kernel” G and filter width $\Delta(x)$. It is generally required that if u is constant throughout the domain then it should not be affected by filtering. This implies that the filter kernel is normalized, i.e.,

$$\int_{(x_0-x)/\Delta(x)}^{(x_1-x)/\Delta(x)} G(s) ds = 1. \quad (3)$$

In case of an infinite domain $x_0, x_1 \rightarrow \mp \infty$ the filter is considered symmetric if $G(s) = G(-s)$ and skewed otherwise. In (2) we restrict to filter kernels that depend explicitly on x

only through the filter width, i.e., we restrict to cases in which the characteristic filter kernels do not explicitly depend on the spatial location. This is not an essential restriction and allows to obtain an insight in the magnitude of commutator errors without being distracted by too much technical detail. More general situations may require G to depend explicitly on x as well and additional contributions arise, e.g., from spatial variations of the skewness. In actual implementations the nonuniformity of the filter may be directly coupled to nonuniformities in the computational grid. Such situations generally require explicit x dependence of G . However, frequently the filter width depends only weakly on x and in this paper we focus particularly on these situations. The restriction to filters with a single x -independent kernel G implies that we focus primarily on turbulent flows well separated from solid bounding walls. As examples one may think of homogeneous turbulence, but also unbounded shear layers such as the turbulent mixing layer²² can be considered in this framework. In Sec. IV we will explicitly evaluate commutator errors and other closure terms using direct numerical simulation results obtained for such a temporal mixing layer. The specific implications of nonuniform filtering near solid boundaries is a topic that requires separate study and will not be included here.

A wide range of filters has been developed over the years. In this paper some well known spatial filters are considered to provide a point of reference. First, the top-hat filter for which the filter kernel is given by

$$G_a^{\text{th}}(s) = \begin{cases} 1 & \text{if } |s-a| \leq \frac{1}{2}, \\ 0 & \text{else.} \end{cases} \quad (4)$$

In this formulation of the top-hat filter the shift-parameter a is by definition restricted to $-\frac{1}{2} \leq a \leq \frac{1}{2}$. Nonzero values of a introduce skewness to this filter while the symmetric top-hat filter is obtained for $a=0$. Next, the Gaussian filter is considered. This filter is characterized by a filter kernel given by

$$G^{\text{Gauss}}(s) = \sqrt{\frac{\alpha}{\pi}} e^{-\alpha s^2}, \quad (5)$$

where commonly the parameter $\alpha=6$. This filter will only be adopted in its symmetric form although it is possible to extend it to a skewed form as well. The Gaussian filter will be used for the construction of higher-order filters, in Sec. IV. A third popular filter is the spectral cutoff in which

$$G^{\text{cutoff}}(s) = \frac{\sin(\pi s)}{\pi s}. \quad (6)$$

In case the integration domain is infinite, the Gaussian and spectral cutoff filters are properly normalized while if a finite domain is considered a compensating factor may readily be added in order for the filter to be normalized as required by (3).

A characteristic property of a spatial filter is its “width” for which different definitions have been proposed in literature.⁶ It is convenient to distinguish between a “basic” and an “effective” filter width, which we specify next. The “basic filter width” is considered the length-scale parameter Δ contained in the formulation of the filter kernel, i.e.,

$G(z, \Delta)/\Delta$. As an example, Δ in the top-hat filter corresponds to the width of its support, while Δ in the Gaussian filter is associated with the width of the Gaussian kernel and Δ in the spectral cutoff filter derives its interpretation in terms of the precise cutoff wave number k_c associated with that filter, i.e., $k_c \Delta = \pi$. The corresponding “effective filter width” is denoted by Δ_e and we specify this through the definition:⁶

$$\frac{1}{\Delta_e(x)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} |h[k, \Delta(x)]|^2 dk = \int_{-\infty}^{\infty} g^2[y, \Delta(x)] dy, \quad (7)$$

where $h(k, \Delta)$ is the Fourier transform of the total filter kernel $g(z, \Delta)$ related to each other via Parseval's equality. This definition applies to all kernels that are square integrable. For such filters we hence arrive at a proper and robust definition for the effective filter width in terms of the basic filter width. If this definition is applied to the top-hat filter we note that $\Delta_e = \Delta$ and the same is observed for the popular spectral cutoff filter. For the Gaussian filter we find $\Delta_e = \Delta \sqrt{2\pi}/\alpha$. For the special choice $\alpha = 2\pi$ we observe that $\Delta_e = \Delta$.

In case a discrete filter is considered, a numerical quadrature rule is applied to the continuous formulation. In one spatial dimension, this implies for the filtered solution at grid-point x_i :

$$\begin{aligned} \bar{u}(x_i) &= \int_{-\infty}^{\infty} g[y - x_i, \Delta(x_i)] u(y) dy \\ &\approx \sum_{j=-n_-}^{n_+} \alpha_{ij} g[x_{i+j} - x_i, \Delta(x_i)] u_{i+j} \equiv \sum_{j=-n_-}^{n_+} w_{ij} u_{i+j}. \end{aligned} \quad (8)$$

In this expression, the discrete filtering of u is represented by a weighted sum of $u_{i+j} = u(x_{i+j})$. The numerical integration covers a sufficiently wide interval $[x_{i-n_-}, x_{i+n_+}]$ and is characterized by integration weights $\{\alpha_{ij}\}$. These integration weights are specific to the quadrature rule that is selected such as the composite trapezoidal rule, Simpson integration, or general higher-order Newton–Cotes methods.^{25,26} The integration weights and filter kernel may be combined in total “filter weights” $\{w_{ij}\}$ where $w_{ij} = \alpha_{ij} g[x_{i+j} - x_i, \Delta(x_i)]$. The definition of the effective filter width in (7) can consistently be applied to discrete filters. Applying the numerical quadrature to (7) leads to

$$\frac{1}{\Delta_e(x_i)} = \sum_{j=-n_-}^{n_+} \alpha_{ij} g^2[x_{i+j} - x_i, \Delta(x_i)]. \quad (9)$$

This provides an effective filter width $\Delta_e(x_i)$ that corresponds directly to the particular numerical realization of the assumed filter. It includes dependencies on the specific filter kernel, underlying grid points, numerical quadrature rule adopted and the selected region to which this numerical integration is applied. With a proper specification of these elements, evaluation on a sufficiently fine grid yields an effective filter width of the discrete filter that converges to the continuous result in (7).

Filtering defined in one spatial dimension can straightforwardly be extended to three spatial dimensions by considering “product filters.” These can be obtained by defining the composition of several one-dimensional filters, i.e., $\mathcal{L}(f)$

$= L_1 \circ L_2 \circ L_3(f) = L_1\{L_2[L_3(f)]\}$, where L_i is a filter used for the x_i direction and f is any solution for which $\mathcal{L}(f)$ is well defined. Each L_i can be characterized by a separate filter width $\Delta_i(\mathbf{x})$ and shift a_i .

We next consider the application of such general three-dimensional filter operators to the equations governing the flow of incompressible fluids. The unfiltered equations are well known and represent the conservation of mass and momentum. These are given by

$$\partial_j u_j = 0, \quad (10)$$

$$\partial_t u_i + \partial_j (u_i u_j) + \partial_i p - \frac{1}{\text{Re}} \partial_{jj} u_i = 0, \quad (11)$$

where we introduced the short-hand notations $\partial/\partial t \rightarrow \partial_t$ and $\partial/\partial x_j \rightarrow \partial_j$ for partial derivatives with respect to time t and spatial coordinate x_j . The velocity in the x_j direction is denoted by u_j , the pressure is given by p , and Re denotes the Reynolds number. Throughout, we will use the summation convention with summation implied over repeated indices in a term. The application of a nonuniform filter $\mathcal{L}$ to the incompressible Navier–Stokes equations yields after some calculation:

$$\partial_j \bar{u}_j = -C_j(u_j), \quad (12)$$

$$\begin{aligned} \partial_t \bar{u}_i + \partial_j (\bar{u}_i \bar{u}_j) + \partial_i \bar{p} - \frac{1}{\text{Re}} \partial_{jj} \bar{u}_i \\ = -\partial_j \tau_{ij} - C_i(u_i) - C_j(u_i u_j) - C_i(p) + \frac{1}{\text{Re}} C_{jj}(u_i), \end{aligned} \quad (13)$$

in which various closure terms have been introduced that will be described in some more detail next.

In case LES is based on commuting filters, only one type of subgrid terms arises, i.e., the divergence of the turbulent stress-tensor τ_{ij} . This contribution has received ample attention in traditional LES literature.^{22,27,28} The turbulent stress-tensor reappears for nonuniform filters and is defined by

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j = [\mathcal{L}, \Pi_{ij}](\mathbf{u}). \quad (14)$$

In this expression the SGS-stress tensor is conveniently written in terms of the commutator bracket involving the filter and the product operators $\Pi_{ij}(\mathbf{u}) = u_i u_j$. In general, the commutator bracket of two operators, A and B , is defined as

$$[A, B](\mathbf{u}) = A \circ B(\mathbf{u}) - B \circ A(\mathbf{u}) = A[B(\mathbf{u})] - B[A(\mathbf{u})]. \quad (15)$$

The commutator errors arising from the nonuniformity of Δ can be expressed conveniently in terms of the commutator bracket as well,¹¹

$$C_j(f) = \overline{\partial_j f} - \partial_j \bar{f} = [\mathcal{L}, \partial_j](f). \quad (16)$$

Finally, also possible temporal- and second-derivative commutator errors are included in (13). These are explicitly defined as

$$C_t(u) = \overline{\partial_t u} - \partial_t \bar{u} = [\mathcal{L}, \partial_t](u), \quad (17)$$

$$C_{jj}(u) = \overline{\partial_{jj}u} - \partial_{jj}\bar{u} = [\mathcal{L}, \partial_{jj}](u) = C_j(\partial_{jj}u) + \partial_j[C_j(u)]. \quad (18)$$

In this paper we restrict ourselves to spatially varying filter widths. Hence, the filter operator commutes with the time-derivative operator and the temporal commutator error $C_t = 0$. Further details regarding temporal commutator errors can be found in Ref. 9.

The commutator bracket defined in (15) satisfies the Leibniz identity,

$$[A, B_1 \circ B_2] = [A, B_1] \circ B_2 + B_1 \circ [A, B_2], \quad (19)$$

which plays a central role in establishing the Poisson-bracket structure in classical mechanics.²⁹ This identity allows to rewrite the second-derivative commutator error in (18) in terms of first-order derivative commutator errors. In case $A = \Pi_{ij}$ and $B_k = \mathcal{L}_k$ for two filters $\mathcal{L}_k$, the Leibniz identity is better known in LES literature as Germano's identity^{3,18} and forms the basis for the successful dynamic modeling procedure.^{2,30} Since Leibniz' identity also applies to the commutator errors $C_j(f)$ and $C_{jj}(f)$, a dynamic modeling procedure can likewise be adopted for their explicit parametrization, thereby locally optimizing specific base models for these commutator errors.

The filtered equations have been written in a specific form, also referred to as the "LES-template." In (12) and (13) we recognize the "Navier–Stokes operator" on the left-hand side, but now applied to the filtered solution $\{\bar{u}_i, \bar{p}\}$. Moreover, instead of the right-hand side being equal to zero, as in (10) and (11), a number of closure terms, also referred to as subgrid terms, have been distinguished to represent all effects of filtering. The filtering with $\mathcal{L}$ has considerably altered the basic structure of the governing equations. We observe that the nonuniformly filtered velocity field is no longer solenoidal. In fact a characteristic commutator error arises in the right-hand side of (12). Likewise, we observe that the strong conservation form of the governing equations was lost as a result of the application of $\mathcal{L}$, i.e., the total flux is no longer in divergence form^{11,12} and material frame indifference is no longer maintained.

As mentioned in the Introduction, the various closure terms either require explicit modeling, or their dynamic importance is sufficiently small for these contributions to be neglected altogether. Since explicit modeling adds (considerably) to the computational effort of a flow simulation and since it may constitute a source of additional error in LES, one has to first carefully assess the need for explicit modeling, separate from the construction of specific models.

The nonuniform filtering of the continuity equation is seen to give rise to an explicit commutator error which corresponds to sources and sinks for mass in the filtered description. It may be difficult to model such a term and one has to properly represent the filtering effect in order to avoid possible instabilities that may arise. If the nonuniformity is sufficiently small, one may consider numerical procedures which retain the solenoidal character of the numerically obtained filtered field. However, if filter nonuniformities are strong, the filtered field will deviate significantly from a solenoidal field and it appears more sensible to introduce explicit commutator-error modeling instead. This area of devel-

opment is quite new in large-eddy simulations and further analysis will be needed in order to arrive at a reliable and robust treatment.

The issue of whether or not to explicitly model some of the closure terms that have arisen in (12) and (13) is closely related to the (local) filter width Δ in relation to typical (viscous) length-scales of the turbulent flow, but also to spatial variations in Δ and the specific smoothing properties of the actual filter operator $\mathcal{L}$. In order for LES to be efficient in turbulent regions, the filter width Δ is set much larger than a local measure for the Kolmogorov length. Typically the filter width is on the order of $1/10$ – $1/100$ of a characteristic mean-flow length scale.^{3,6,31,32} In these cases the SGS-stress-tensor τ_{ij} certainly requires explicit modeling, or representation by the implicit dissipative and dispersive properties of an upwind spatial discretization as in the MILES approach.³³ Various SGS models are available, see, e.g., Refs. 6, 22, and 27. Whether the new commutator errors need to be explicitly modeled as well or whether these closure terms can safely be neglected is very much dependent on the variability of the filter width. In the following section we estimate the size of the convective flux commutator error $C_j(u_i u_j)$ and compare its scaling in terms of Δ and Δ' with that of the turbulent stress-tensor contributions, in case general high-order filters are adopted. In the sequel, if we refer to "the" commutator error it will be implied that we refer to $C_j(u_i u_j)$ unless explicitly stated otherwise.

III. ORDER OF MAGNITUDE ESTIMATES OF SUBGRID TERMS FOR SKEWED AND HIGH-ORDER FILTERS

In this section we determine the dominant scaling of the commutator errors for various general filters. First we turn to symmetric second-order filters, then we consider effects of skewness and finally we introduce higher-order filters. Subsequently, we estimate the magnitude of the turbulent stress contributions. It will be shown that both types of subgrid terms can be reduced arbitrarily by raising the order of the filter to a sufficiently high value. In fact, both subgrid contributions display identical leading-order scaling with the nonuniform filter width and its derivatives. Consequently, for nonuniform filter widths both contributions may require explicit modeling. In case the filter width is constant, only the turbulent stress contributions remain. Hence, commutator errors can only be avoided independently by properly controlling the gradients in Δ . It is not possible to reduce the commutator errors separately by merely adhering to specialized higher-order filters.

To determine the order of magnitude of the commutator errors one may explicitly evaluate $\partial_x \bar{f}(x)$ in one spatial dimension (see also Refs. 7, 8, and 12). After some calculation the following expression for the commutator error is obtained:

$$C_x(f)(x) = -\Delta'(x) \int_{(x_0-x)/\Delta(x)}^{(x_1-x)/\Delta(x)} sG(s)f'[x+\Delta(x)s]ds \\ + \frac{1}{\Delta(x)} \left[1 + (y-x_0) \frac{\Delta'(x)}{\Delta(x)} \right] G\left(\frac{y-x}{\Delta(x)}\right) f(y) \Big|_{y=x_0}^{x_1}. \quad (20)$$

As noted most explicitly in Ref. 12, the commutator error consists of two parts; an interior part and a boundary term. The latter term arises since principally filtering cannot be extended beyond the boundaries of the flow domain.³⁴ For common filters, identified in the preceding section, this contribution is zero or negligible if x is sufficiently separated from the boundary. The interior contribution to the commutator error arises directly from the nonuniform filter width, as expressed by the leading Δ' factor. In the remainder of this paper we will restrict ourselves to the interior part of the commutator-error and consider $x_0 \rightarrow -\infty$ and $x_1 \rightarrow \infty$. This is appropriate for the inhomogeneous turbulent mixing layer flow studied here.

The scaling of the interior part of the commutator error with filter width can be inferred from Taylor expansion, provided the solution is sufficiently smooth. If one introduces the coordinate transformation $s=(y-x)/\Delta(x)$ in (2) one obtains after some calculation

$$C_x(f)(x) = -\Delta'(x) \int_{-\infty}^{\infty} sG(s)f'(x+\Delta(x)s) ds \quad (21)$$

$$= -\Delta'(x) \int_{-\infty}^{\infty} sG(s) \left[f'(x) + s\Delta(x)f''(x) + \frac{1}{2}s^2\Delta^2(x)f'''(x) + \dots \right] ds \quad (22)$$

$$= -\sum_{r=1}^{\infty} \frac{1}{(r-1)!} \Delta' \Delta^{r-1} M_r \frac{\partial^r f}{\partial x^r}, \quad (23)$$

where M_r denotes the r th moment of the filter, defined as

$$M_r = \int_{-\infty}^{\infty} s^r G(s) ds. \quad (24)$$

Since we consider normalized filters the zeroth moment $M_0 = 1$. In the sequel we restrict to filters for which all moments M_r with $r > 0$ exist. It should be remarked that the well known spectral cutoff filter does not satisfy this condition; in particular, for the spectral cutoff filter the even order moments beyond second order do not exist. We hence exclude the traditional spectral cutoff filter from the discussion. This does not mean that the cutoff filter would be of no value to large-eddy simulation. For all bounded solutions u , the cutoff filtered solution $\bar{u}$ is well defined, which in particular holds for bounded periodic solutions such as occur in homogeneous turbulence for which spectral methods and filters are ideally suited. Moreover, one may consider restricting the cutoff filter to a (large but) finite domain. After renormalizing the kernel appropriately to compensate for this truncation of the domain, generally a second-order filter arises in view

of (25). In this section we will for convenience also assume that the solutions have continuous derivatives of all orders and convergent Taylor expansions.

The smoothing properties of general filters can be characterized to some degree by the effect of filtering on polynomials. For convenience in what follows we formalize this and introduce an N th order filter by requiring,

$$M_r = \delta_{r0} \quad \text{for } r = 0, \dots, N-1, \quad (25)$$

where δ_{ij} denotes the Kronecker delta. Such N th order filters leave polynomials of degree $N-1$ invariant. Actual examples of higher-order filters may be constructed in different ways. Specific polynomial kernels on a compact support of width Δ may be obtained,¹⁸ which give rise to higher-order filters. Alternatively, high-order filters may be constructed by suitably combining basic filters such as the top-hat or Gaussian filters at different length scales.¹⁷ Either way, such higher-order filters are automatically formulated in terms of the basic filter width Δ . It is important to notice that if one keeps Δ fixed in this class of filters then the effective filter width at order N , denoted by $\Delta_e(N)$, can be shown to decrease (rapidly) with increasing N . Paradoxically, one may simultaneously refer to the width of the specific higher-order filter as being fixed and equal to Δ or interpret the increase in the order of the filter at fixed Δ in terms of the reducing effective filter-width $\Delta_e(N)$. The latter interpretation is more appealing in order to emphasize that at fixed Δ the filtering becomes less and less effective with increasing N and, for the filters considered by us, approaches the identity operator in the limit. In fact, the limiting identity operator leaves all modes invariant which corresponds to its Fourier transform being equal to unity for all wave numbers. Correspondingly, the effective wave number as defined in (7) is zero, in line with the limiting behavior of $\Delta_e(N)$ mentioned above.

To illustrate the effect of higher-order filters we consider the scaling of $|\bar{u} - u|$ with the local filter width Δ in case u is an infinitely smooth solution with a globally convergent Taylor expansion. Application of higher-order filters gives rise to

$$|\bar{u} - u| = \Delta^N \left| \sum_{r=N}^{\infty} \frac{M_r}{r!} \partial_x^r u(x) \Delta^{r-N}(x) \right| \\ \leq \Delta^N \sum_{r=N}^{\infty} \left| \frac{M_r}{r!} \partial_x^r u(x) \right| \Delta^{r-N}(x). \quad (26)$$

To establish the dominant scaling $\sim \Delta^N$ for Δ sufficiently small, the series in the upper bound of (26) needs to be considered in more detail. We observe that the convergence radius of this series depends on $|M_r \partial_x^r u(x)/r!|$. Different cases may be distinguished. We will first discuss the simplest case in which M_r and $\partial_x^r u$ are bounded separately, for all x and r . Then we turn to filters for which M_r is an increasing function of r , but $M_r/r!$ decreases monotonically, and finally we further relax the restrictions and consider solutions u for which $\partial_x^r u$ may become unbounded as $r \rightarrow \infty$.

The simplest and most restrictive evaluation of the upper-bound in (26) arises if M_r and $\partial_x^r u(x)$ are bounded separately. In that case we may write

$$|\bar{u} - u| = \Delta^N \left| \sum_{r=N}^{\infty} \frac{M_r}{r!} \partial_x^r u(x) \Delta^{r-N}(x) \right| \leq \mathcal{M}_N \mathcal{U}_N \Delta^N \sum_{m=0}^{\infty} \frac{1}{(m+N)!} \Delta^m, \quad (27)$$

where we introduced

$$\mathcal{M}_N = \max_{r \geq N} |M_r|; \quad \mathcal{U}_N = \max_{r \geq N} \max_x |\partial_x^r u(x)|. \quad (28)$$

The series in the upper bound on the right-hand side of (27) is a simple power series which can be shown to have an infinite radius of convergence and in particular the upper bound for $|\bar{u} - u|$ tends to zero as N becomes large, for all bounded Δ . Not only does $|\bar{u} - u|$ tend to zero as N becomes large, but also other filter effects, e.g., the subgrid stresses. Consequently, for this class of higher-order filters it is possible to arrive at conclusions regarding the subgrid stress based on the filter moments, and to infer the dominant scaling behavior in the mathematical limit $\Delta \rightarrow 0$. Note that this restriction of sufficiently small filter-width Δ is essential. In fact, Δ should be smaller than the smallest relevant length scale contained in the unfiltered solution in order for the dominant scaling behavior to apply quantitatively. This situation differs completely from the typical LES setting in which the filter width is chosen such that it corresponds to an inertial range length scale. In that case a restriction of the analysis to only the low-order moments can be misleading. In such practical LES settings the actual filter width is not small enough and one has to be careful with the significance of predictions involving only the low-order moments since these primarily relate to low frequency information in the solution. However, the dominant scaling in the particular academic situation $\Delta \rightarrow 0$ does provide some first impression about the contributions arising from explicit high-order filtering. This is complemented by a full database analysis to which we turn in the following section.

In the proof of (24) it is essential that all moments of the filter are bounded. This property may be verified for filters with a compact support and bounded kernel. However, various popular filters do not have this property. For example, the moments of the Gaussian filter are such that M_r keeps increasing with r . For this filter one can, however, also establish a simple upper-bound estimate for $|\bar{u} - u|$ which is slightly more restrictive on the filter-widths Δ for which it holds. In fact, for the Gaussian filter one may establish that $M_r/r!$ decreases rapidly and monotonously with r . For higher-order filters which share this property one may readily show

$$|\bar{u} - u| = \Delta^N \left| \sum_{r=N}^{\infty} \frac{M_r}{r!} \partial_x^r u(x) \Delta^{r-N}(x) \right| \leq \frac{|M_N|}{N!} \mathcal{U}_N \Delta^N \sum_{m=0}^{\infty} \Delta^m. \quad (29)$$

This also establishes leading-order deviations of $O(\Delta^N)$ in case $\Delta \ll 1$. However, instead of the stronger result in (24) we now observe that the upper-bound estimate involves the geometric series which is convergent only provided $\Delta < 1$. So, while the assumption that all M_r are bounded leads to an upper bound in (24) which contains a series that is convergent for all Δ , the weaker assumption that $M_r/r!$ decreases monotonously gives rise to an upper-bound estimate that is valid only for a finite range of filter widths. Since this analysis of the scaling behavior only applies to the academic limiting case where $\Delta \ll 1$ anyway, the finiteness of the convergence interval does not affect the validity of the result.

Returning to (26) we may further relax the restrictions and also incorporate solutions for which $\partial_x^r u$ is not bounded for all r . We assume that $|\partial_x^r u| \leq u_0/(\delta^r)$ for a suitable velocity-scale u_0 and length-scale δ . If δ is small enough then higher-order derivatives grow with r and may become unbounded as $r \rightarrow \infty$. In this case one may estimate

$$|\bar{u} - u| \leq u_0 \sum_{r=N}^{\infty} \frac{|M_r|}{r!} \left(\frac{\Delta(x)}{\delta} \right)^r. \quad (30)$$

As before, in (27), under the assumption that $|M_r| \leq \mathcal{M}_N$ for all $r \geq N$ we may simply obtain an upper-bound estimate that contains a series that is globally convergent, thus establishing the leading-order Δ^N for this case. For the situation in which M_r increases with r , the estimates need to be considered slightly more carefully. If the increase of M_r is not more rapid than $|M_r| \leq m_0(r/l)!c^r$ with positive constants m_0 , c , and integer l , we find

$$|\bar{u} - u| \leq u_0 m_0 \sum_{r=N}^{\infty} \frac{(r/l)!}{r!} \left(\frac{c\Delta(x)}{\delta} \right)^r. \quad (31)$$

Hence, if $l \geq 2$ the series converges globally, while a series with finite convergence radius arises as $l=1$. In either case ($l=1$ or $l \geq 2$) the dominant order N scaling in the mathematical limit $\Delta \rightarrow 0$ is established.

In terms of (25) the symmetric top-hat filter and the Gaussian filter are second-order filters, while the asymmetric top-hat filter, G_a^{th} with $a \neq 0$, is formally only first order, i.e., only normalized. This illustrates that nonzero skewness decreases the order of the corresponding symmetric filter. Moreover, higher-order filters may be constructed which have several odd and even moments equal to zero. For symmetric filters all odd moments are zero since the kernel is an even function. However, skewed higher-order filters in which a controlled number of odd moments are zero by construction may be developed systematically as well. There exist various constructions for specific higher-order filters. Not all these constructions lead to filters that damp all modes in a signal; examples may be obtained in which the Fourier transform of the filter kernel assumes values larger than unity for a limited range of wave numbers. This corresponds to actual amplification of the corresponding modes instead of their

desired reduction. However, it is not too difficult to arrive at classes of higher-order filters that do display proper reduction for all modes in a solution. Examples of such higher-order filters with proper damping properties, corresponding to $N > 2$ have originally been proposed in the context of LES in several papers by Geurts^{13,18} and Vasilyev *et al.*¹⁵

Next the general expression for the commutator error in (23) will be used to discuss the influence of the specific filter. We first consider symmetric filters. In this case all odd moments M_{2r-1} , $r \geq 1$ are equal to zero. The lowest order contribution in (23) may arise at $r=2$ and the commutator error is of order $O(\Delta' \Delta)$. This estimate for the commutator error applies to common second-order filter such as the symmetric top-hat or Gaussian filters and has been derived before in literature.^{8,12,13} Next, we turn to skewed filters. In this case the odd moments M_{2r-1} are nonzero and the lowest order contribution to the commutator error may arise at $r=1$. Thus, skewness formally reduces the order of the filter and increases the scaling of the commutator error to $O(\Delta')$.

One has to realize that, although filters can be strictly asymmetric, it is well possible that the lowest order contributions to the commutator error remain very small. Effects of skewness on the commutator error become apparent only in case the lowest order odd moments M_{2r-1} become sufficiently large. For example, the filters considered in Ref. 8 are strictly skewed filters in physical space. However, in illustrations found in this reference the odd moments were negligible compared to the even moments M_{2r} and overall the filters approximately corresponded to symmetric filters. For the skewed top-hat filter considered in this paper G_a^{th} the first and second moments are given by $M_1 = a$ and $M_2 = \frac{1}{12} + a^2$. Hence, effects of skewness are expected to become relevant if the shift a is large enough. As an indication $|M_1| \approx M_2$ for $1/10 \geq |a| \geq 1/2$.

The expression for the commutator error as given in (23) suggests the possibility of directly controlling its magnitude by considering higher-order filters as introduced above. By requiring that certain moments M_r identically vanish, the leading-order contribution to the commutator error can be controlled explicitly. Specific high-order filters serving this purpose were proposed by Van der Ven.¹⁴ In view of (23) all N th order filters have the property that the implied commutator error reduces to $O(\Delta' \Delta^{N-1})$. This would allow to neglect the commutator-error contributions from the filtered LES equations, simply by turning to an appropriate higher order of filtering. However, the dominant scaling behavior of the commutator error is of no consequence by itself. Rather, one has to incorporate the dominant scaling of the divergence of the turbulent stress-tensor as well, before anything more definite can be established. We turn to this next.

In order to establish the dominant scaling of the turbulent stress contributions we proceed analogous to the above derivation for the commutator error. The one-dimensional SGS-stress tensor is given by $\tau = \overline{u^2} - \bar{u}^2$ for which one readily obtains

$$\tau(x) = \overline{u^2}(x) - \bar{u}^2(x) \quad (32)$$

$$= \int_{-\infty}^{\infty} G(s) \left(\sum_{r=0}^{\infty} \frac{1}{r!} \Delta^r s^r \partial_x^r u^2 \right) ds - \left\{ \int_{-\infty}^{\infty} G(s) \left(\sum_{r=0}^{\infty} \frac{1}{r!} \Delta^r s^r \partial_x^r u \right) ds \right\}^2, \quad (33)$$

in which we used expressions for $\overline{u^2}$ and $\bar{u}$ arrived at by a Taylor series expansion similar to (22) (see also Refs. 18 and 35). This expression can be simplified to

$$\begin{aligned} \tau(x) = & \sum_{r=0}^{\infty} \frac{M_r}{r!} \Delta^r \partial_x^r u^2 - \sum_{r=0}^{\infty} \left(\frac{M_r}{r!} \right)^2 \Delta^{2r} (\partial_x^r u)^2 \\ & - 2 \sum_{q=0}^{\infty} \sum_{r=q+1}^{\infty} \frac{M_q M_r}{q! r!} \Delta^{q+r} \partial_x^q u \partial_x^r u. \end{aligned} \quad (34)$$

For smooth solutions u and filters for which all moments exist, one may readily show that the series in (34) converge for all Δ , following the same reasoning as in (27). This implies that the dominant scaling behavior which arises in the limit $\Delta \rightarrow 0$ is well defined and may be used to characterize the effect of higher-order filtering for the turbulent stress tensor. However, the filtered solution still contains some small-scale contributions on scales of order Δ and hence terms such as $(M_r/r!) \Delta^r \partial_x^r u^2$ may not be small for a range of r values. Therefore, although the limiting dominant scaling behavior is a meaningful aspect of the turbulent stress, the impression obtained from the leading-order terms should be interpreted with some care. In particular, the leading-order terms typically do not constitute an accurate subgrid model for relatively large filter widths. Moreover, the leading-order terms alone may induce explicit instabilities in the modeled equations as occurs, e.g., with the so-called nonlinear or Clark model for τ .

For an N th order filter the scaling behavior of the turbulent stress tensor displays characteristic dominant terms. These can be inferred from (34) as

$$\tau(x) = \frac{M_N}{N!} (\partial_x^N u^2 - 2u \partial_x^N u) \Delta^N + O(\Delta^{N+1}). \quad (35)$$

From (35) we observe that $\tau \sim \Delta^N$ for general N th order filters, in case $N \geq 2$. Consequently, the relevant flux $\partial_x \tau$ scales with terms of $O(\Delta^N)$ as well as terms of $O(\Delta' \Delta^{N-1})$. We observe that the dominant formal scaling behavior is identical to that established above for the commutator error with a subdominant correction of $O(\Delta^N)$. In the special case $N=1$, the first term in (35) is identically zero in view of the property $\partial_x u^2 = 2u \partial_x u$. For these filters the SGS stress is thus unaffected by a nonzero first moment M_1 and, although $N=1$ the turbulent stress tensor scales as $O(\Delta^2)$. This is formally one order in Δ smaller than the corresponding commutator-error at $N=1$.

Taking the derivative of the first term in (35) in order to obtain an impression of the subgrid flux, one observes a contribution which contains Δ' next to a contribution which corresponds to the classical subgrid flux formulated in terms of the local filter width. This raises the question whether successful models for τ that were developed for spatially uni-

form filters will remain accurate when nonuniform filters are used. At least, classical models for τ which are formulated in terms of the local filter width will induce both types of subgrid fluxes, i.e., the “explicitly nonuniform contributions” containing Δ' and the remaining terms. However, for nonuniform filters, accuracy of a subgrid model should now also imply an accurate description of the explicitly nonuniform contributions, next to the proper characterization of τ itself. To what extent popular models such as Smagorinsky³⁶ or Bardina²³ already fulfill both these wishes is a central problem which deserves further attention.

In actual large-eddy simulations the numerical representation of the solution introduces a grid truncation next to the smooth filtering. For finite-volume, finite-difference, or finite-element methods the spatial discretization may be approximated to some extent by a second “implicit” filter which is denoted by ℓ with filter width δ . In addition, the finite spatial resolution in any simulation induces an element of grid truncation in ℓ . This truncation obviously limits the strict approach to the identity operator associated with high-order smooth filters as we will discuss next. The total stress tensor corresponding to the composition of ℓ and L obeys

$$[\ell \circ L, \Pi](u) = [\ell, \Pi](L(u)) + \ell([L, \Pi](u)). \quad (36)$$

For convenience, we assume L to be of order N and ℓ of order n . As far as the scaling of the turbulent stress tensor is concerned, we have in that case $[L, \Pi](u) = O(\Delta^N)$ and so $\ell([L, \Pi](u)) = \ell(O(\Delta^N)) = O(\Delta^N)$. Likewise $L(u) = \bar{u} = u + O(\Delta^N)$ which leads to $[\ell, \Pi](L(u)) = O(\delta^n) + O(\Delta^N)$. If $\delta \ll \Delta$ the implicit filter associated with the spatial discretization effectively corresponds to the identity operator for all scales up to Δ . This large separation of scales between the resolved scales, the larger subfilter scales and the grid-truncation scales allows one to focus on the $O(\Delta^N)$ turbulent stress tensor and to ignore specific numerical aspects. Conversely, if $\delta \approx \Delta$ or if the order of L becomes very high with correspondingly small effective filter width, no significant separation of scales is present. Such may arise in actual coarsely resolved large-eddy simulations and the lower order filter among L and ℓ may become the dominant one. In such cases one has to reckon with significant discretization effects. Moreover, the total filter effects no longer gradually reduce to zero with an increase in the order of the smooth filter for all length scales, but are limited by the grid truncation of the implicit filter instead. An increase in the number of zero moments of L will correspond to a convergence to the identity operator only in the grid-truncated frequency range which is inherent to any simulation. In the sequel we will concentrate on the nonuniform filtering problem and consider (local) filter widths sufficiently larger than the grid spacing on which the numerical solution is available.

Although the use of higher-order filters allows additional control over the size of the subgrid terms, the dominant scaling of both the commutator error as well as the divergence of the turbulent stress tensor with Δ and its derivatives is formally identical if $N \geq 2$. For $N=1$ we even observe that the commutator error is formally larger than the SGS flux. Judging from these order of magnitude estimates, this suggests that if in a certain flow the turbulent stress contributions

require explicit modeling, one should also consider incorporating explicit modeling for the commutator errors. It appears to make little sense to model one of the subgrid terms and ignore the other class of subgrid contributions which are formally of equal order of magnitude.

The order of magnitude estimates provide only a fairly rough indication of the dynamic importance of the individual subgrid contributions. In fact, rather than controlling the size of the commutator errors by increasing the order of the filter as suggested before in literature, the control of the spatial variations in Δ appears to allow another method of separately influencing the size of the SGS flux relative to that of the commutator errors. If Δ' can be kept sufficiently small, it is conceivable that the terms with the lowest order scaling in Δ have a (very) small “pre-factor” which can even imply that only the next order terms, i.e., the turbulent stress related contributions only, require explicit treatment. In order to analyze these aspects we turn to an *a priori* analysis of the various subgrid terms in the following section and determine the actual size of the commutator errors and turbulent stress contributions in developed turbulent mixing.

IV. A PRIORI ANALYSIS OF COMMUTATOR ERRORS IN TURBULENT MIXING FLOW

In this section, data of DNS of turbulent flow in a temporal mixing layer will be used to quantify the magnitude of commutator errors and SGS fluxes for a variety of filter width nonuniformities and filter specifications. In particular, for skewed as well as higher-order filters the size of the closure terms will be determined and specific trends will be interpreted in view of the analysis presented in the preceding section. We first describe the DNS, then introduce some measures with which the closure terms will be quantified and finally present *a priori* results which establish the magnitude of the terms in relation to, e.g., filter width, skewness, and order of the filter.

A. Description of DNS and filter widths

For the *a priori* analysis of the commutator errors we consider turbulent flow in a temporal mixing layer. We evaluate data presented in Ref. 22. The governing equations are solved in a cubic geometry of side ℓ which is set equal to four times the wavelength of the most unstable mode according to linear stability theory. Periodic boundary conditions are imposed in the streamwise (x_1) and spanwise (x_3) direction, while in the normal (x_2) direction the boundaries are free-slip walls. The initial condition is formed by mean profiles corresponding to constant pressure, $u_1 = \tanh(x_2)$ for the streamwise velocity component and $u_2 = u_3 = 0$. Superimposed on the mean profile are two- and three-dimensional perturbation modes obtained from linear stability theory. The DNS data were obtained at a spatial resolution of 192^3 grid cells, employing a fourth-order accurate spatial discretization scheme in combination with explicit Runge–Kutta time stepping. A full description may be found in Ref. 22.

The filter widths that will be considered are kept constant in the x_1 and x_3 directions while in the x_2 direction we allow for significant variations in Δ . Specifically, the filter

width is reduced considerably near the centerline where the flow is most unsteady and displays rapid, large-amplitude variations. We parametrize the filter-width variations by the following two-parameter family:

$$\Delta_1 = \Delta_3 = \Delta_r, \quad \Delta_2(x_2) = \Delta_r(1 - \alpha e^{-(\beta x_2/\ell)^2}). \quad (37)$$

The reference filter width Δ_r is taken equal to $\ell/16$, corresponding to the evaluation of LES described in Ref. 22. In the definition of the nonuniform filter width $\Delta_2(x_2)$, the parameter α controls the ratio between the minimal filter-width and Δ_r , i.e., α measures the “depth” of the filter width modulation. In addition, the parameter β controls the width of the region of the flow domain in which the filter width varies significantly. The maximal value of α considered here is $\alpha = 3/4$ which corresponds to a minimal filter width $\Delta_{\min} = \Delta_r/4 = \ell/64$ which is equal to three grid cells in the DNS grid. In Fig. 1 different nonuniform filter-width variations are shown alongside snapshots of the evolving flow. By varying α and β and specific properties of the filter such as skewness and order, a systematic assessment of the commutator errors can be made.

B. Measures for the closure terms

To quantify the dynamic effects of the closure terms we concentrate on the decomposition of the nonuniformly filtered convective flux. This decomposition follows from the application of a nonuniform filter operator $\mathcal{L}$ to the convective terms in the momentum equations, i.e.,

$$\overline{\partial_j(u_i u_j)} = \partial_j(\bar{u}_i \bar{u}_j) + \partial_j \tau_{ij} + C_j[u_i u_j], \quad (38)$$

where we distinguish a mean, SGS-flux, and commutator-error contribution on the right-hand side of (38), respectively. Since the filter width is considered nonuniform only in the x_2 direction the commutator error $C_j(u_i u_j)$ reduces to $C_2(u_i u_2)$.

To quantify the magnitude of the various fluxes in (38) the L_2 norm is considered, which for a field f is defined as

$$\|f\|^2 = \frac{1}{|\Omega|} \int_{\Omega} f(\mathbf{x})^2 d\mathbf{x}. \quad (39)$$

The domain of integration Ω can coincide with the entire flow-domain ℓ^3 and $d\mathbf{x} = dx_1 dx_2 dx_3$, but for some quantities we will restrict the integration to the homogeneous directions x_1 and x_3 and adapt Ω accordingly. This allows to identify the variation of the field f in the normal direction.

Next to the L_2 norm of the individual contributions in (38) we also consider the transport equation for the resolved kinetic energy $\bar{E}$. After some calculation one may derive

$$\begin{aligned} \varepsilon &= -\partial_t \bar{E} = -\partial_t \left(\int_{\Omega} \frac{1}{2} \bar{u}_i \bar{u}_i d\mathbf{x} \right) \\ &= \varepsilon_{\text{mean}} + \varepsilon_p + \varepsilon_{\text{visc}} + \varepsilon_{\text{SGS}} + \varepsilon_{\text{CE}}, \end{aligned} \quad (40)$$

where we identified different contributions defined as follows:

$$\varepsilon_{\text{mean}} = \int_{\Omega} \left(\bar{u}_i \partial_j \bar{u}_i \bar{u}_j - \frac{1}{2} \bar{u}_i \bar{u}_i \partial_j \bar{u}_j \right) d\mathbf{x}, \quad (41)$$

FIG. 1. Contours of the spanwise vorticity of the temporal mixing layer at (a) $t=20$, (b) $t=50$, and (c) $t=80$. Superimposed on these figures are the nonuniform filter-width variations Δ_2 as a function of x_2 for the case $\alpha = 3/4$ and $\beta=5$ (dotted), $\beta=10$ (solid), and $\beta=30$ (dashed).

$$\varepsilon_p = \int_{\Omega} (\bar{u}_i \partial_i p) d\mathbf{x}, \quad (42)$$

$$\varepsilon_{\text{visc}} = -\frac{1}{\text{Re}} \int_{\Omega} (\bar{u}_i \partial_j \partial_j \bar{u}_i) d\mathbf{x}, \quad (43)$$

$$\varepsilon_{\text{SGS}} = \int_{\Omega} (\bar{u}_i \partial_j \tau_{ij}) d\mathbf{x}, \quad (44)$$

$$\varepsilon_{\text{CE}} = \int_{\Omega} \left(\bar{u}_i \mathcal{C}_j(u_i u_j) - \frac{1}{2} \bar{u}_i \bar{u}_j \mathcal{C}_j(u_j) \right) d\mathbf{x}. \quad (45)$$

These individual terms denote the mean convective contribution, the pressure contribution, the viscous dissipation, the SGS contribution, and the effect of the commutator error, respectively. The contribution due to the pressure ε_p was shown to be negligible at the low Mach number ($M=0.2$) considered in the DNS.²² In case Ω is the entire domain (ℓ^3) the mean dissipation $\varepsilon_{\text{mean}}$ is zero in view of the boundary conditions. As mentioned above, by restricting the integration domain to the homogeneous x_1 and x_3 directions, the definitions (40)–(45) reduce to local dissipation—or transport terms.

The evaluation of the various closure terms and diagnostics from the DNS data employs different filters and filter widths. Moreover, different numerical methods may be adopted in the postprocessing of the data. The basic methods adopted in this paper are formally second-order accurate. For the numerical integration the trapezoidal rule has been applied. If data are required at locations not contained in the DNS grid, linear interpolation is used to obtain approximate values. Finally, derivatives are approximated using second-order central finite differences with mesh-spacing $\Delta_r/4$ which is equal to the minimal filter width incorporated. Next to the basic combination of second-order methods we also repeated part of the analysis using fourth-order accurate methods. We observed small changes in specific results. However, turning to such higher-order methods does not lead to alterations in the conclusions that may be drawn. Therefore, in the sequel we will only present results obtained using the second-order methods.

After these preparations we next present the results of the *a priori* analysis, concentrating on the decomposition (38) and the kinetic energy dissipation rate (40). First, we turn to symmetric second-order filters and consider different nonuniform filter widths to provide a point of reference. Then we consider effects of skewness in combination with the top-hat filter. Finally, we introduce a class of high-order filters, based on the Gaussian filter, and explicitly calculate the size of the SGS fluxes and the commutator errors for increasing filter order.

C. Magnitude of commutator errors for second-order symmetric filters

In Fig. 2 results are shown in case the symmetric top-hat filter G_0^{th} is applied to the field at $t=60$ and the nonuniform filter width is determined by $\alpha=3/4$ and $\beta=10$. For the L_2 norms only the results from the field in the streamwise direction, i.e., originating from $\partial_j(u_1 u_j)$, are shown. The L_2 norms corresponding to $\partial_j(u_2 u_j)$ and $\partial_j(u_3 u_j)$ display similar behavior and are not shown. The graphs in Fig. 2(a) indicate that the L_2 norm of the commutator error is about an order of magnitude smaller than the SGS flux $\partial_j \tau_{ij}$ for this specific case. The SGS flux itself is again one order of magnitude smaller than the mean convective flux $\partial_j(\bar{u}_1 \bar{u}_j)$. The latter finding is consistent with previous observations made by Vreman *et al.*³⁷ for this flow.

FIG. 2. (a) L_2 norms of the decomposition (38) in the streamwise direction and (b) contributions to the resolved kinetic energy dissipation of the mean convective flux (dash-dotted), SGS flux $\partial_j(\tau_{ij})$ (dashed), and commutator error (solid). We use $\alpha=3/4$, $\beta=10$, and consider the field at $t=60$. The variations of the filter width as a function of x_2 are depicted by the dotted line.

Regarding the contributions in Fig. 2(b) the SGS flux represents almost all the dissipation of resolved kinetic energy. In addition, the net positive and negative contributions originating from the mean convective flux are seen to approximately cancel, confirming that $\varepsilon_{\text{mean}}=0$ if integrated over the entire flow domain. Finally, the contribution from the commutator error is found to be positive and therefore a dissipative term in this case. The location of maximum local contribution to the commutator-error dissipation coincides approximately with the location where Δ' is maximal, consistent with the basic analysis in the preceding section. The local contribution to the SGS-dissipation ε_{SGS} is maximal near the centerline of the flow. Similarly to the L_2 norm, the maximum contribution to the commutator error dissipation ε_{CE} is about an order of magnitude smaller than the maximum of SGS contribution.

To further classify the type of contributions to the dynamics of the resolved kinetic energy we next distinguish the

FIG. 3. The explicit dissipation (solid) and production (dashed) contributions to the resolved kinetic energy dissipation due to (a) the SGS flux and (b) the commutator error.

explicit sources of dissipation and production. The positive ε^+ and negative contributions ε^- for the SGS flux are defined as

$$\varepsilon_{\text{SGS}}^+(x_2) = \int_{\Omega} \max(0, \bar{u}_i \partial_j \tau_{ij}) dx_1 dx_3,$$

$$\varepsilon_{\text{SGS}}^-(x_2) = \int_{\Omega} \min(0, \bar{u}_i \partial_j \tau_{ij}) dx_1 dx_3. \quad (46)$$

Likewise, we can formulate $\varepsilon_{\text{CE}}^+$ and $\varepsilon_{\text{CE}}^-$ for the commutator error. Production ε^- is often associated with “backscatter” in literature. In Fig. 3 the production and dissipation corresponding to the SGS fluxes and commutator errors are shown. In both cases the dissipation is larger than the production, resulting in a net dissipation as already shown in Fig. 2(b). The ratio between the total production and total dissipation, defined as the integral over x_2 of $\varepsilon^\pm(x_2)$, is observed to be about the same for the SGS fluxes and the commutator errors.

FIG. 4. The L_2 norm of the commutator error in the streamwise direction at $t=60$: (a) $\alpha=1/4$ (dashed), $1/2$ (dotted), and $3/4$ (solid) with β fixed to 10; (b) α fixed to $3/4$ and $\beta=5$ (dash-dotted), 10 (solid), 30 (dashed), and 60 (dotted).

Next we compare different nonuniform filter widths $\Delta_2(x_2)$. In view of (23), the second-order top-hat filter G_0^{th} should give rise to a commutator error that scales with $\Delta\Delta'$. The influence of Δ' on the commutator errors can be controlled by varying the parameters α and β . In Fig. 4 the L_2 norms are shown for different combinations of α and β . An increase in either α or β corresponds to an increase in Δ' . Correspondingly, the larger and spatially more localized variations in the filter width lead to considerable increases in the commutator errors. This may readily be inferred from Figs. 4(a) and 4(b).

In complex turbulent flows one may wonder which strategy of spatially varying Δ is best. On the one hand one may select a fairly gradual transition between a region of large/small filter width to a nearby region of small/large filter width. One may think of a case as represented by $\beta=5$ in Fig. 4(b). Then, Δ' is small and so is the commutator error; no explicit modeling of this contribution appears to be required. This seems to be the most favorable strategy, but one has to realize that it is also computationally the most expensive. A gradual transition requires a wide transition region

which may be wasteful in terms of number of grid points. On the other hand, if a relatively sharp transition is considered, e.g., illustrated by $\beta=60$, the derivative Δ' may become sufficiently large to lead to a commutator error which may no longer be neglected. In fact, the commutator error can locally become as important as the SGS fluxes and correspondingly the commutator error should be explicitly modeled. Depending on whether or not adequate models for the commutator-error contributions can be formulated, one may be tempted to adopt the “safer” more expensive option or the more efficient option which requires a commutator-error model. The proper resolution of the problem how best to adapt Δ is at the heart of developing LES for complex flows and requires further research to which a forthcoming paper will be devoted.

We next proceed by considering the effect of skewness of the filter and subsequently turn to higher-order filters. In the latter case we will explicitly compare the magnitude of the commutator errors with that of the SGS fluxes for increasing order of filtering.

D. Skewness and commutator errors

An efficient implementation of nonuniform filters gives rise to skewed filters in a very natural way. Consider filtering at a grid-location x_i . In one dimension this can be obtained by integrating over the interval $[x_{i-m}, x_{i+n}]$ where m and n are suitable integers. Even if the filter corresponds to a “symmetric” choice of points around x_i , i.e., $m=n$, the nonuniformity of the grid in physical space will imply asymmetry and non-zero skewness. Skewed filters are virtually unavoidable close to solid walls while in other flow-regions skewness arises quite naturally from grid-non-uniformities, if one uses this grid-based implementation. Strictly speaking, grid and filter-width nonuniformities do not have to correspond directly to each other and nonuniform filters can also be defined on uniform grids, as is considered here. Either way, this sketch illustrates that typical filters in complex flow domains are likely to be skewed and effects of skewness deserve to be studied in detail.

In the preceding section it has been shown that skewness of a filter can have a considerable effect on the size of the commutator error. Skewness implies a decrease of the order of the filter compared to the associated symmetric case. For filters that are second order at zero skewness, nonzero skewness leads to a commutator error of order $O(\Delta')$. Here, we will explicitly calculate the size of the commutator errors for the skewed top-hat filter G_a^{th} defined in (4). For simplicity, we consider the case of constant skewness, which is adequate to illustrate the main effects.

In Fig. 5 the L_2 norm and local energy transport $\varepsilon(x_2)$ of the commutator error and the SGS fluxes are shown as function of the shift-parameter a . From the series expansion of the SGS stress it was concluded that this term was not affected by a nonzero first moment. In Fig. 5(a) we observe indeed that the size of the SGS flux is largely unaffected by the value of the shift $a=M_1$. This is in sharp contrast with the L_2 norm of the commutator error for which a significant increase is observed with increasing $|a|$ as predicted by the analytical estimates obtained in the preceding section.

FIG. 5. (a) L_2 norms of the SGS fluxes and commutator errors in the stream-wise direction and (b) contributions to the resolved kinetic energy dissipation at $t=60$ for the asymmetric top-hat filter in case $a=0$ (solid), $a=0.25$ (dash-dotted), $a=0.50$ (dashed), and $a=-0.50$ (dotted). The upper set of curves correspond to the SGS fluxes, and the lower set of curves denote the effect of the commutator errors.

Additional illustrations of skewness in relation to the commutator error can be observed in Fig. 5(b), where the local contributions $\varepsilon_{\text{SGS}}(x_2)$ and $\varepsilon_{\text{CE}}(x_2)$ are shown. The SGS contributions are quite unaffected by the skewness of the filter, while the commutator-error effect increases with $|a|$. In case skewed filters are applied the commutator-error contribution to the resolved kinetic energy dissipation loses its symmetry across the centerline at $x_2=0$. The resulting commutator-error effect can even change sign, either above or below the centerline depending on a , which indicates that not only the size but also the dynamical consequences of the commutator error may depend considerably on the skewness. It may be shown that symmetric filters give rise to dissipative effects and nonzero skewness is associated with additional dispersive contributions.³⁸

Finally, we observe that in certain regions of the flow domain the effects of the SGS fluxes and the commutator errors are of comparable magnitude in case the skewness is sufficiently large. So, unlike most cases involving symmetric

second-order filters, strongly skewed lower order filters imply that one can no longer ignore the explicit inclusion of commutator errors in the subgrid modeling.

In the following paragraphs higher-order filters will be considered and the decrease of the commutator error with increasing filter order will be compared with that of the SGS fluxes. First the construction of a specific class of higher-order filters will be described. Estimates for the commutator error and SGS fluxes will subsequently be discussed.

E. Construction of higher-order filters

In literature various classes of higher-order filters have been proposed. Vasilyev *et al.*¹⁵ constructed a class of filters, which was later extended to complex geometries by Marsden *et al.*¹⁹ and by Haselbacher and Vasilyev.²⁰ These filters are based on a nonuniform grid to achieve nonuniform filtering. In our application here, we would prefer to be able to adopt a wide range of different nonuniform filter widths without having to change the grid each time, i.e., achieve a level of independence between filter width and grid nonuniformities. To arrive at such a formulation the so-called Daubechies construction is used.¹⁷

The construction of Daubechies filters relies on a wavelet-type transformation of a general base filter $G_0(s)$. We require that all moments M_r , $r \geq 0$ of the base-filter $G_0(s)$ exist and that the base filter is properly normalized, i.e., $M_0=1$. The desired higher-order filter-kernel $G_N(s)$ is expressed as

$$G_N(s) = \sum_{j=0}^{n-1} d_j G_0\left(\frac{s}{j+1}\right), \quad (47)$$

where d_j are appropriate constants, which will be determined next taking (25) into account. We note that the filter kernel G_N has a much wider support compared to the original base filter since s is divided by $j+1$.

We selected the Gaussian filter (5) as base filter and restrict ourselves here to symmetric filters. By definition the higher-order filter kernel inherits the symmetry properties of the base filter and the odd moment M_{2r+1} of G_N are zero. We define $n=N/2$ in (47). The requirements for higher-order filters (25) give rise to the following system of equations for the unknown coefficients $\{d_j\}$:

$$\delta_{i0} = \int s^{2i} \sum_{j=0}^{n-1} d_j G_0\left(\frac{s}{j+1}\right) ds = M_{2i} \sum_{j=0}^{n-1} d_j (j+1)^{2i+1}, \quad (48)$$

for $i=0, \dots, n-1$ and M_{2i} are the moments of the base-filter. For second-order base filters $M_{2i} \neq 0$ and by definition $M_0 \equiv 1$. Hence (48) can be multiplied by M_{2i}^{-1} and an $n \times n$ linear system $\mathbf{A}\mathbf{d}=\mathbf{b}$ for $\mathbf{d}=[d_0, d_1, \dots, d_{n-1}]$ results where $\mathbf{A}$ and $\mathbf{b}$ are defined as

$$A_{ij} = (j+1)^{2i+1}, \quad b_i = \delta_{i0}, \quad i, j = 0, \dots, n-1. \quad (49)$$

It can be shown that the matrix $\mathbf{A}$ is invertible. For various n explicit construction of the higher-order filters can be obtained using, e.g., Maple and in Table I resulting coefficients are given for several higher-order filters.

TABLE I. Resulting coefficients $\{d_j\}$ for several lower order filters.

N	$\{d_j\}$
4	$\{\frac{4}{3}, -\frac{1}{6}\}$
6	$\{\frac{3}{2}, -\frac{3}{10}, \frac{1}{30}\}$
8	$\{\frac{8}{5}, -\frac{2}{5}, \frac{8}{105}, -\frac{1}{140}\}$

The moments M_{2i} depend on the specific choice for the base filter. However, the coefficients $\{d_j\}$ follow from $\mathbf{A}\mathbf{d}=\mathbf{b}$ from which these moments have been removed; consequently the coefficients $\{d_j\}$ are independent of the specific choice of the symmetric base filter. This construction can also be developed for asymmetric filters in which case $A_{ij}=(j+1)^{i+1}$ and $n=N$. In Fig. 6 some resulting higher-order filters are depicted. As the desired filter order is increased the filter kernel is seen to develop characteristic changes of sign which imply that the realizability conditions for the turbulent stress tensor are no longer maintained.³⁹

Numerically, the integrals are approximated using the trapezoidal rule. Following (8) the discrete filter can be formulated as

$$\bar{u}_i = \sum_{j=-n_-}^{n_+} w_{ij} u_{i+j}, \quad (50)$$

where the filter weights w_{ij} are given by

$$w_{ij} = \frac{x_{i+1} - x_{i-1}}{2} \frac{1}{\Delta(x_i)} G_N\left(\frac{x_j - x_i}{\Delta(x_i)}\right). \quad (51)$$

In this approach the numbers n_- and n_+ should be chosen fairly large in order for the moments M_r , $r=1, \dots, N-1$ to be accurately captured. We selected $n_-=n_+=96$, i.e., integrate over all points in the grid. The discrete moments

FIG. 6. Higher-order filters, Gaussian second order (solid), fourth order (dotted), and eighth order (dashed).

$$M_r \approx \sum_{j=-n_-}^{n_+} w_{ij} \left(\frac{x_{i+j} - x_i}{\Delta_i} \right)^r \quad (52)$$

were found to be smaller than 10^{-5} , for all moments $r = 1, \dots, N-1$, up to $N=8$ for the cases considered. Hence, up to eighth-order filtering is achieved in this way.

F. Magnitude of SGS fluxes and commutator errors as function of filter order

In Sec. III it was shown that an N th order filter gives rise to a commutator error which scales with $O(\Delta' \Delta^{N-1})$. Also, for $N \geq 2$ the SGS-stress τ_{ij} scales with $O(\Delta^N)$, which leads to a SGS-flux $\partial_j \tau_{ij}$ with contributions of $O(\Delta^N)$ and $O(\Delta' \Delta^{N-1})$. Hence, in regions where Δ' is sufficiently large, both SGS flux and commutator error display identical dominant scaling in Δ controlled by the order of the filter. Consequently, both contributions may require explicit subgrid modeling in such regions. To further illustrate this, we will next extend the dominant scaling analysis with the calculation of the actual size of the SGS flux and commutator errors in turbulent mixing. We will use the symmetric high-order Daubechies filters with nonuniform filter widths constructed above.

In Fig. 7 the local contributions ε_{SGS} and ε_{CE} are shown for several higher-order filters. First, we compared the Gaussian filter with the symmetric top-hat filter. These two second-order filters are shown to yield only minor differences, confirming findings in Ref. 39. In Fig. 7 the strong reduction of the contribution of both the SGS flux and the commutator error with increasing filter order can be observed. Roughly speaking the maximal local SGS-flux contribution decreases by about 30% for every increase of the filter order by 2. The size of the commutator-error contribution is seen to be reduced slightly more rapidly with increasing order of the filter. When N changes from 2 to 4 the maximum commutator-error contribution decrease by about 35% and by an additional 50% when N is increased to 6. We hence clearly observe that both the SGS-flux and commutator-error contributions reduce in a fairly comparable way with increasing order of filtering. The specific implementation of the higher-order filters used here may induce some inaccuracy in the evaluation of the higher-order cases. This does not permit a further quantitative evaluation of the observed behavior. However, the general trends are sufficiently strong to illustrate the predicted decrease of *both* contributions as N increases, which was the central point of this analysis.

The use of higher-order filters not only influences the dominant scaling of the subgrid terms but it may also affect the construction of acceptable subgrid models. It is not necessarily true that SGS models which are accurate in combination with ordinary second-order filters work equally well for higher-order filters. For example, the standard Smagorinsky model^{36,27} contains an explicit scaling with Δ^2 which also carries over to the popular dynamic model.³⁰ In addition, the well known gradient or Clark model is explicitly based on filters with a nonzero second moment.^{22,24} In case higher-order filters are adopted to try to reduce the explicit

FIG. 7. Contribution to the dissipation of the resolved kinetic energy caused by (a) the SGS flux and (b) by the commutator error at $t=60$ for higher-order filters, second-order Gaussian (solid), fourth order (dotted), and sixth order (dashed). Also depicted are the results obtained with the second-order top-hat filter (circles).

influence of the commutator error, it appears unavoidable that one should also incorporate corresponding changes in the basic model assumption for the SGS stresses, e.g., correct the model to comply with the theoretical scaling. Similarity models such as Bardina's model²³ or Leray's model⁴⁰ do not require such an explicit alteration; the proper dominant scaling is already contained in the definition of these models.

The analysis in this and the preceding section has indicated that skewness of a filter, which is often unavoidable, can have a strong influence on the size of the commutator error relative to the SGS flux. Moreover, sufficiently rapid variations in the local filter width may induce local situations in which the commutator error is no longer negligible compared to the SGS fluxes. Finally, the use of higher-order filters does not offer an independent control over the size of either type of subgrid terms. Hence, in various situations or for the sake of retaining appropriate efficiency in LES of complex flows, one has to resort to explicitly developing

specific models for the commutator error. We will present an analysis of similarity type commutator-error models in the following section to illustrate this point.

V. EXPLICIT MODELING OF THE COMMUTATOR ERROR

In this section we first formulate explicit models for the commutator errors.¹³ Subsequently, results of *a priori* testing will be discussed, where special attention will be given to the quality of the proposed models in case skewed filters are applied.

A. Similarity commutator-error models

Motivated by the close capturing of turbulent stresses by similarity SGS models, we will illustrate the explicit commutator-error modeling by extending the similarity idea accordingly. We concentrate on Bardina's similarity concept and the associated gradient approximation.

The first commutator-error model (CE model) extends the Bardina model²³ to also include the commutator error. For any nonlinearity f the similarity CE model arises by applying the definition of the exact commutator error to the available filtered solution. In particular, the exact commutator error corresponding to f may be written as $C_j(f)(\mathbf{u}) = [\mathcal{L}, \partial_j] \circ f(\mathbf{u})$. Consequently, the similarity model may be defined as

$$C_j^{\text{sim}}(f)(\bar{\mathbf{u}}) = [\mathcal{L}, \partial_j] \circ f(\bar{\mathbf{u}}) = \overline{\partial_j f(\bar{\mathbf{u}})} - \partial_j \overline{f(\bar{\mathbf{u}})}. \quad (53)$$

In this formulation $f(\bar{\mathbf{u}})$ denotes the operator f acting on filtered quantities. Since f is still arbitrary (53) represents the similarity formulation for general nonlinearities, e.g., also those associated with exponential dependencies such as in some combustion models.^{41–43} For the commutator error corresponding to the quadratic nonlinearity in the convective fluxes we obtain

$$C_j^{\text{sim}}(\Pi_{ij})(\bar{\mathbf{u}}) = [\mathcal{L}, \partial_j] \circ \Pi_{ij}(\bar{\mathbf{u}}) = \overline{\partial_j(\bar{u}_i \bar{u}_j)} - \partial_j \overline{\bar{u}_i \bar{u}_j}, \quad (54)$$

which will be investigated next.

The similarity model for the commutator error contains a number of additional explicit applications of the filter operator. These are computationally expensive and an alternative can be obtained using Taylor expansions. This gives rise to the gradient CE model. It shows close resemblance to the gradient SGS model,²⁴ except that here also the first-order contribution is incorporated in order to accommodate skewed filters. The derivation of the gradient CE model proceeds analogous to the derivation of (23) and results in

$$C_j^{\text{gradient}}(f)(\bar{\mathbf{u}}) = -\{M_{k1}(\partial_j \Delta_k) \partial_k f(\bar{\mathbf{u}}) + M_{k2} \Delta_k (\partial_j \Delta_k) \partial_k^2 f(\bar{\mathbf{u}})\}, \quad (55)$$

where the summation over k runs from 1 to 3 and M_{kr} is the r th moment of the filter applied in the k th direction. The first and second moments of the filter make this model sensitive to the actual filter that was adopted. For the *a priori* testing of these models the (skewed) top-hat filter G_a^{th} will be used, for which we obtained $M_1 = a$ and $M_2 = \frac{1}{12} + a^2$.

Further analogies between the SGS fluxes and the commutator errors may be exploited to extend existing SGS models to CE models. For example, generalized similarity models may involve (approximate) inversion,^{44,45} or regularization principles such as Leray's formulation.⁴⁰ Moreover, the commutator error formally obeys Germano's identity² which may be formulated as follows. If a test-filter $\mathcal{L}_{\text{tf}}$ is introduced next to $\mathcal{L}$ then the following identity may be verified:

$$[\mathcal{L}_{\text{tf}} \circ \mathcal{L}, \partial_j](u) = [\mathcal{L}_{\text{tf}}, \partial_j] \circ \mathcal{L}(u) + \mathcal{L}_{\text{tf}} \circ [\mathcal{L}, \partial_j](u). \quad (56)$$

This identity represents Leibniz's rule for the commutator-error bracket and may allow the dynamic determination of possible additional parameters in assumed basic CE models, similar to dynamic modeling approaches which were found successful for the SGS stress.³⁰

The explicit evaluation of an additional CE model can be computationally expensive. Therefore, it may be an appealing idea to return to the basis of the nonuniform filtering and combine the modeling of the commutator error with that of the SGS terms. So, instead of distinguishing two separate closure problems which may have separate subgrid models, we may directly consider the modeling of the full convective-flux contribution, i.e., $\partial_j(u_i u_j) - \partial_j(\bar{u}_i \bar{u}_j)$.⁴⁶ One may easily verify that

$$\begin{aligned} \overline{\partial_j(u_i u_j)} &= \overline{\partial_j(\bar{u}_i \bar{u}_j)} + \{\overline{\partial_j(u_i u_j)} - \overline{\partial_j(\bar{u}_i \bar{u}_j)}\} \\ &= \partial_j(\bar{u}_i \bar{u}_j) + [\mathcal{L}, \partial_j \circ \Pi_{ij}](\mathbf{u}). \end{aligned} \quad (57)$$

The similarity closure of this formulation arises directly as before

$$\begin{aligned} [\mathcal{L}, \partial_j \circ \Pi_{ij}](\mathbf{u}) &\rightarrow [\mathcal{L}, \partial_j \circ \Pi_{ij}](\bar{\mathbf{u}}) \\ &= [\mathcal{L}, \partial_j] \circ \Pi_{ij}(\bar{\mathbf{u}}) + \partial_j [\mathcal{L}, \Pi_{ij}](\bar{\mathbf{u}}) \\ &= C_j^{\text{sim}}(\Pi_{ij})(\bar{\mathbf{u}}) + \partial_j \tau_{ij}^{\text{Bard}}(\bar{\mathbf{u}}), \end{aligned} \quad (58)$$

where $\tau_{ij}^{\text{Bard}} = [\mathcal{L}, \Pi_{ij}](\bar{\mathbf{u}})$ is Bardina's similarity model. Not surprisingly, we observe that the similarity modeling of the separate closure problems corresponds fully to the similarity modeling of the full convective-flux contribution. By adopting the same modeling assumptions for both the SGS stress and commutator error the combined model can be implemented at reduced computational cost. A similar situation arises in relation to Leray regularization.⁴⁷ This regularization closure not only implies a model for the SGS stress but also for the commutator error and the combined evaluation can be shown to be not more expensive than in case uniform filters are considered.

In the remainder of this section we will consider results of *a priori* testing of the two explicit similarity CE models. Other models mentioned above and their performance in actual LES will be discussed elsewhere.

B. A priori testing of CE models

For the *a priori* testing of the CE models we incorporate a number of different quantities. We will consider the correlation of the models with the exact commutator errors $C_j(u_i u_j)$ as well as with $C_j(u_j)$, as a function of time. More-

TABLE II. Correlation results for the gradient and similarity commutator-error models for symmetric filters.

t	Gradient model				Similarity model			
	$C_j(u_1 u_j)$	$C_j(u_2 u_j)$	$C_j(u_3 u_j)$	$C_j(u_j)$	$C_j(u_1 u_j)$	$C_j(u_2 u_j)$	$C_j(u_3 u_j)$	$C_j(u_j)$
0	0.61	0.68	0.01	0.82	0.99	0.99	0.95	0.99
10	0.53	0.54	-0.08	0.65	0.94	0.93	0.92	0.95
20	0.62	0.56	0.20	0.70	0.93	0.85	0.91	0.94
30	0.76	0.63	0.60	0.82	0.95	0.85	0.91	0.95
40	0.78	0.75	0.69	0.88	0.95	0.90	0.95	0.96
50	0.74	0.73	0.71	0.87	0.95	0.90	0.95	0.96
60	0.75	0.73	0.72	0.90	0.94	0.88	0.93	0.96
70	0.76	0.75	0.71	0.91	0.92	0.88	0.91	0.96
80	0.74	0.77	0.71	0.90	0.93	0.89	0.92	0.95
90	0.80	0.80	0.74	0.90	0.93	0.90	0.93	0.96
100	0.80	0.83	0.81	0.92	0.94	0.93	0.96	0.96

over, we compare the L_2 norms and the contributions to the dissipation of the resolved kinetic energy $\varepsilon_{CE}(x_2)$ for the various models. We adopt the (skewed) top-hat filter G_a^{th} and first turn to the symmetric case. Afterwards, we will discuss the performance of the similarity models for the skewed case.

In Table II the correlations are shown for the gradient—and the similarity model with filter-width variations corresponding to $\alpha=3/4$ and $\beta=10$. The similarity model displays almost perfect correlation during all transitional and turbulent stages of the development of the temporal mixing layer. Regarding the gradient model we notice somewhat lower correlations. During the initial stages ($0 \leq t \leq 30$) the correlation in the transitional regime displays a slight decrease, compared to the average values, for $C_j(u_1 u_j)$, $C_j(u_2 u_j)$, and $C_j(u_j)$ while $C_j(u_3 u_j)$ shows virtually no correlation in this regime. Beyond $t=30$ the mixing layer reached nonlinear saturation and more or less steady, quite high levels of correlation are observed. In Table II the gradient model shows an average correlation of 0.74 for $C_j(u_1 u_j)$ and 0.89 for the commutator error in the continuity equation $C_j(u_j)$. The similarity model performs slightly better, 0.92 for $C_j(u_1 u_j)$ and 0.96 for $C_j(u_j)$. From this correlation analysis we conclude that both models are well capable of capturing the important spatial variations in the commutator error that arise in this flow. This corresponds closely to similarly high correlation observed between these similarity models and the turbulent stress tensor.²²

The predictions of both CE models for the L_2 norms and for ε_{CE} are collected in Fig. 8. Again, we use $\alpha=3/4$ and $\beta=10$ and consider the turbulent field at $t=60$. Only the L_2 norms for $C_j(u_1 u_j)$ are shown; the results corresponding to the normal and spanwise directions as well as results related to $C_j(u_j)$ lead to similar conclusions. From Fig. 8(a) it can be observed that the similarity model tends to underpredict the commutator error, while the gradient model overpredicts the commutator error. The results for ε_{CE} in Fig. 8(b) indicate that the similarity CE model is not sufficiently dissipative. The contribution due to the gradient model does correspond very well with the exact commutator error dissipation.

FIG. 8. (a) The L_2 norm of the commutator-error $C_j(u_1 u_j)$ and (b) contribution to the dissipation of the resolved kinetic energy as predicted by the exact commutator error (solid), gradient CE model with $M_1=0$, $M_2=1/12$ (dashed), and similarity CE model (dotted) for the symmetric top-hat filter.

We next turn to an analysis for skewed filters. Whereas the predictions of both similarity models appeared quite accurate for symmetric filters, the situation is quite different for strongly skewed filters. Results at maximal skewness $a=1/2$ for the correlations are given in Table III. In the developed regime $t \geq 30$ the gradient model shows a correlation which is slightly larger than obtained for the similarity model; 0.67 compared to 0.61 for $C_j(u_1 u_j)$ and 0.75 compared to 0.65 for $C_j(u_j)$. Both models correlate less well with the exact commutator error compared to the symmetric case (cf. Table II).

Although a correlation in the range of 0.6–0.75 may still be considered reasonable, the predictions for the L_2 norms and ε_{CE} are rather inaccurate. Both models appear unable to properly capture these quantities for the strongly skewed case, as shown in Fig. 9. We also included the symmetric gradient CE model using $M_1=0$ and $M_2=1/12$. The symmetric gradient model leads to a strong underprediction of the commutator error. In case the gradient model with properly adjusted moments is used the gradient model exaggerates the commutator error. The L_2 norm as predicted by the similarity

TABLE III. Correlation results for the gradient and similarity commutator-error models for the nonsymmetric top-hat filter with $a=\frac{1}{2}$, $\alpha=3/4$, and $\beta=10$. The gradient model includes both moments explicitly, i.e., $M_1=a$, $M_2=\frac{1}{12}+a^2$.

t	Gradient model				Similarity model			
	$C_f(u_1u_j)$	$C_f(u_2u_j)$	$C_f(u_3u_j)$	$C_f(u_j)$	$C_f(u_1u_j)$	$C_f(u_2u_j)$	$C_f(u_3u_j)$	$C_f(u_j)$
0	0.78	0.82	0.40	0.90	0.58	0.59	0.36	0.57
10	0.79	0.76	0.50	0.87	0.63	0.57	0.42	0.56
20	0.74	0.72	0.61	0.84	0.65	0.59	0.52	0.56
30	0.73	0.75	0.71	0.83	0.67	0.64	0.54	0.65
40	0.72	0.75	0.72	0.83	0.65	0.65	0.58	0.63
50	0.67	0.73	0.72	0.80	0.63	0.60	0.59	0.66
60	0.57	0.67	0.65	0.76	0.59	0.55	0.58	0.59
70	0.53	0.64	0.61	0.68	0.63	0.52	0.50	0.61
80	0.50	0.71	0.69	0.70	0.68	0.57	0.58	0.65
90	0.50	0.75	0.75	0.70	0.68	0.59	0.65	0.69
100	0.45	0.76	0.74	0.66	0.69	0.60	0.62	0.69

model is seen to be somewhat too low but clearly predicts the L_2 norm with greater accuracy in this example.

The predictions for $\varepsilon_{CE}(x_2)$ are shown in Fig. 9(b). Again, the both gradient model realizations are quite unacceptable. Moreover, especially the gradient model with proper values for the moments completely misses regions with a net negative contribution to the resolved kinetic energy dissipation. The similarity model at least resolves some of the production as well as dissipation although large discrepancies remain.

In summary, both explicit CE models produce reasonable results in combination with the symmetric top-hat filter, but their parametrization of the commutator error in combination with strongly skewed filters appears inadequate. Especially the gradient model fails noticeably for the skewed case. In contrast, the similarity model maintains some accuracy in the prediction of the size and dissipative nature of the commutator error. Further development and *a posteriori* testing of explicit commutator-error models is required in order to reliably apply LES in cases with large, strongly skewed and spatially localized filter-width variations. The alternative consists of trying to set up the numerical treatment such that such filter-width nonuniformities are largely avoided. In the following section we collect some concluding remarks and discuss the conditions under which explicit commutator-error modeling may be unavoidable.

VI. CONCLUDING REMARKS AND DISCUSSION

In this paper we presented results of research into the commutator error in LES. This closure term arises in case a filter with nonuniform filter width is applied to the Navier–Stokes equations. The dynamic consequences of the commutator error and its explicit modeling received comparably little attention in literature. However, for the application of LES to practical situations in which complex flow phenomena are present in a complex flow domain, the use of a filter width which depends on space and/or time is considered very advantageous.⁸ An investigation of the associated commuta-

FIG. 9. (a) The L_2 norm of the commutator error $C_f(u_i u_j)$ and (b) contribution to the dissipation of the resolved kinetic energy as predicted by the exact commutator error (solid), gradient CE model with $M_1=0$, $M_2=1/12$ (dash-dotted), gradient CE model with $M_1=a$ and $M_2=\frac{1}{12}+a^2$ (dashed), and similarity CE model (dotted) for the skewed top-hat filter G_a^{th} with $a=\frac{1}{2}$.

tor error is a prerequisite before filters with nonuniform filter width can be applied with confidence. We addressed this issue in a number of ways as will be sketched next.

We first identified all commutator errors that arise from nonuniformly filtering the incompressible Navier–Stokes equations. It was shown that all closure terms can be expressed as commutator brackets involving the filter operator and either the product or differentiation operator. Consequently, these terms share a number of important properties with the Poisson bracket in classical mechanics.¹⁸ This observation allows to develop dynamic subgrid modeling for all closure terms, i.e., including the commutator errors.

The main commutator error arises from filtering the convective flux $\partial_j(u_i u_j)$. It can be expressed as

$$C_f(u_i u_j) = [\mathcal{L}, \partial_j](\Pi_{ij})(\mathbf{u}) = \overline{\partial_j u_i u_j} - \partial_j \overline{u_i u_j} \quad (59)$$

and should be directly compared with the SGS fluxes $\partial_j \tau_{ij}$ involving the turbulent stress-tensor $\tau_{ij} = [\mathcal{L}, \Pi_{ij}](\mathbf{u})$. Using Taylor expansions the influence on the commutator error

arising from the filter width Δ , its spatial derivative $\nabla[\Delta(\mathbf{x})]$ or the order of the filter, has been established. For general N th order filters the commutator error was shown to scale with $\Delta' \Delta^{N-1}$. For common filters such as the symmetric top-hat and Gaussian filters this implies a scaling with $\Delta' \Delta$. The scaling even reduces to $O(\Delta')$ for first-order filters which arise from skewed versions of popular second-order filters. From a similar analysis the SGS-stress tensor τ_{ij} scales with $O(\Delta^N)$ in case $N \geq 2$ and with $O(\Delta^2)$ for $N=1$. This yields an SGS flux $\partial_j \tau_{ij}$ that scales with a formally dominant contribution of $O(\Delta' \Delta^{N-1})$ and subdominant term of $O(\Delta^N)$. In case $\|\nabla[\Delta(\mathbf{x})]\|$ is sufficiently large this scaling analysis indicates that both the commutator error and the SGS flux behave in the same way. In fact, this analysis suggests that the use of higher-order filters does not allow an *independent* control over the commutator error compared to the SGS flux, as was hinted at before.^{14,15} Moreover, for skewed filters, additionally with sharp variations in filter width the explicit modeling of both closure terms appears unavoidable.

Using DNS data of the temporal mixing layer²² the magnitude of the commutator error and the SGS flux was explicitly calculated in order to complement the dominant scaling analysis. The use of turbulent flow data allowed for a quantitative comparison between the dynamical importance of the commutator error and the SGS stress. The effect of skewness of the filter on the commutator error showed to be considerable in certain cases, consistent with the observation that the order of a filter is reduced by one if the kernel is skewed. For the commonly adopted top-hat and Gaussian filters this is especially important because the SGS stress is unaffected by a nonzero first moment M_1 . The *a priori* analysis reveals that strongly skewed filters induce a commutator error which becomes locally as important as the SGS stress and thus both closure terms would require explicit modeling. Likewise, the commutator error requires explicit modeling in case Δ' becomes sufficiently large. Finally, the influence of the order of the filter on the magnitude of the closure terms was determined and the global trends were found to be in line with the scaling analysis.

Since very little developments have been made in the explicit modeling of commutator errors, it is natural to consider under what conditions these terms can safely be neglected. Unlike suggestions made in literature that this can be achieved by adhering to higher-order filters, an *independent* control over the size of the commutator errors compared to the SGS fluxes is obtained only by properly restricting spatial variations of the filter width. Keeping the gradient of the filter width small presents itself as a favorable strategy for avoiding the commutator error. Unfortunately, with this option one remains quite close to the uniform filter-width situation and this does not offer a flexible and computationally effective adaptation to complex flows in complex domains. It appears therefore that explicit modeling of commutator errors may open up important new possibilities for LES.

To illustrate this alternative, two specialized models for the commutator error were proposed and analyzed. We considered the similarity model and the approximating gradient model. In combination with symmetric filters the similarity

model was found to be quite accurate, showing a correlation of about 90%. This model displayed, however, too low contributions to the dissipation of the resolved kinetic energy. The computationally more efficient gradient model showed a correlation of about 80% and successfully captured the dissipation of resolved kinetic energy $\varepsilon_{CE}(x_2)$. In case skewed filters were applied both these basic models were shown to fail considerably which indicates that more effort has to be put into the development of accurate commutator-error models. Good opportunities exist by extending dynamic modeling or following the revisited regularization approaches.⁴⁰ Future research will be devoted to these developments and will include the application of specific commutator-error models in actual large-eddy simulations on nonuniform grids. The dynamic adaptation of the filter width is one of the central issues that will be investigated. An implementation in terms of finite element discretizations will be considered and applied to vortex dominated flows of aerodynamic interest, e.g., in which slender and coherent vortices develop behind an airplane wing.

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