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Lagrangian dynamics of commutator errors in large-eddy simulation

Fedderik van der Bos

Department of Applied Mathematics, Faculty of Electrical Engineering Mathematics and Computer Science, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Bernard J. Geurts

Department of Applied Mathematics, Faculty of Electrical Engineering Mathematics and Computer Science, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands and Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

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In large-eddy simulations of turbulent flow only the flow structures with length scales larger than the local filter width Δ are explicitly resolved. We analyze the dynamic effect associated with spatial variations in the filter width. With the introduction of such a nonuniform filter width a number of additional closure terms emerges, generally referred to as commutator errors. The dynamic effect of the commutator errors is shown to correspond to the apparent local creation or destruction of turbulent flow scales, depending on, respectively, a decrease or an increase in Δ along the flow path. This Lagrangian context suggests significant correlation between the material derivative of the filter width and the production or dissipation of kinetic energy due to the commutator error. This is confirmed by novel *a priori* analysis of turbulent mixing. An explicit Lagrangian model for the commutator error in the momentum equations is proposed. Additionally, the dynamic effect of a skewed filter on the commutator error is investigated. It is shown that skewed filters induce both dissipative and dispersive behaviors, which are explicitly retained in the new Lagrangian model. © 2005 American Institute of Physics. [DOI: 10.1063/1.1941364]

I. INTRODUCTION

For the efficient computation of turbulent flows various reduced flow simulation strategies have been proposed in recent years. One of the most promising of these reduced flow simulation strategies is large-eddy simulation (LES). In LES the turbulent flow field is decomposed into large $\bar{\mathbf{u}}$ and small scales $\mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}}$ using a low-pass spatial filter with an associated externally specified filter width Δ . The spatial filtering allows computation with grid spacing on the order of the filter width Δ instead of the Kolmogorov scale $\eta \ll \Delta$. The latter resolution is required in order to resolve all details of a turbulent flow in the so-called direct numerical simulation (DNS). The application of the filter effectively removes the small or subfilter-scale (SFS) [In LES literature the term subgrid-scale contributions is often found instead of SFS. Throughout this paper we will adhere to SFS which is somewhat more correct] flow features from the formulation. The dynamical effects of the SFS scales on the resolved scales are mainly incorporated through the SFS stress $\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$, which is replaced by a SFS model in order to close the equations. The modeling of the SFS stress has received ample attention over the years and a wide range of models have been proposed.¹⁻⁴

In recent years the demand has become stronger for LES to be extended to realistic flow situations as encountered, e.g., in industry, aerodynamics, and local weather prediction. To efficiently extend the capabilities of LES to such complex flow situations we require the filter width to become dependent on space (and possibly also on time). This introduces a local nonuniform filter width $\Delta(\mathbf{x})$ (Refs. 5 and 6) which has a number of obvious benefits. A nonuniform filter width al-

lows to zoom in on turbulent parts of the flow domain and locally resolve more turbulent flow scales, while in regions with comparably quiescent flow a wider filter width may be adopted which allows computations on a coarser and hence cheaper grid.

The introduction of a nonuniform spatial filter also has some complicating drawbacks. In fact, a nonuniform filter width induces a number of additional closure terms, generally referred to as commutator errors.⁵⁻⁹ These commutator errors express the noncommutation between filtering and differentiation. For a field f we may define the commutator error as

$$C_j(f) = \overline{\frac{\partial f}{\partial x_j}} - \frac{\partial \bar{f}}{\partial x_j}, \quad (1)$$

where x_j denotes the j th Cartesian coordinate and the overbar represents the spatial filter. Compared with the SFS stress τ_{ij} , the commutator error received little attention in literature. However, the commutator error can become dynamically important in case the local variations in the filter width are strong enough. Such strong variations in Δ may be necessary, e.g., near solid boundaries¹⁰ or in case sharp gradients need to be resolved only in part of the flow domain such as near detached shear layers or when studying the turbulent decay of trailing vortices behind an airplane.¹¹ It is essential to understand and model the fundamental properties of these terms in the LES equations in order to arrive at an efficient and successful extension of LES toward problems of realistic complexity. Most studies of the commutator error that were reported in literature relied on an analytical evaluation of the

commutator error^{5,6,9,12} or on *a priori* investigations using DNS data.⁷

In this paper an explicit Lagrangian interpretation of the dynamics of commutator errors is provided which directly suggests a corresponding SFS model. We examine the effect of commutator errors on the transport of resolved kinetic energy. It will be shown that the commutator error can be associated with the apparent local creation and destruction of resolved flow features in case the filter width is decreased or increased along a flow path, respectively. As a consequence, the amount of kinetic energy which is locally resolved varies when filter-width variations are encountered along a flow path. The Lagrangian interpretation suggests to model the commutator error in terms of the material derivative of the filter width. This model may capture both spatial as well as temporal variations in the filter width. We will formulate the explicit Lagrangian commutator-error model and test it against other commutator-error models (CE models) that are based on similarity assumptions instead.⁶⁻⁸

The type of nonuniform filter in the definition of the commutator error explicitly affects the type of dynamic contributions of these terms. We will investigate both the commonly used symmetric filters as well as skewed filters. Symmetry or skewness of a filter is associated with the filter kernel being an even function or not. The use of skewed filters is sometimes unavoidable, e.g., when the local filter width is defined in terms of a fixed number of grid intervals. This implies smaller filter width in case the grid is locally refined, but also implies skewness of the filter. Earlier studies have shown that the dynamic effect of the commutator error becomes significantly larger when skewed filters are used.⁷ In this paper both the dispersive and dissipative effects associated with filter skewness^{5,6,13} will be included explicitly in the Lagrangian modeling. *A priori* testing of these models using simulation data of turbulent mixing establishes that explicitly accounting for skewness is essential in order to maintain acceptable accuracy.

The organization of this paper is as follows. In Sec. II we introduce general nonuniform filtering and identify all the commutator errors encountered in the nonuniformly filtered Navier-Stokes equations. In Sec. III we consider the dynamic effect of a nonuniform filter width on the evolution of the resolved kinetic energy. We propose, in addition, a new explicit parametrization for the transport of resolved kinetic energy. In Sec. IV we describe the *a priori* testing of this new model. Section V contains the results of *a priori* testing of the proposed Lagrangian model for the commutator error as arises in the momentum equations, and establishes the role of filter skewness. Finally, in Sec. VI some concluding remarks are collected.

II. NONUNIFORM FILTERING AND COMMUTATOR ERRORS

In this section, we introduce the governing equations for incompressible flow and apply general nonuniform filtering. Next to variations in the filter width, we allow explicit skewness of the filter. This may be motivated by the occurrence of complex physical phenomena or arising from complex flow

domains, e.g., associated with a large-eddy treatment of flow near solid boundaries, near sharp interfaces, or close to corners in the flow domain. We identify all closure terms and specifically extract the commutator errors that arise in the nonuniformly filtered Navier-Stokes equations. This creates a point of reference for the analysis and modeling in subsequent sections.

To arrive at the large-eddy equations for turbulent flow, we start from the unfiltered Navier-Stokes equations governing incompressible flow. These equations represent conservation of mass and momentum and are given in dimensionless form by

$$\partial_j u_j = 0, \quad (2)$$

$$\partial_t u_i + \partial_j (u_i u_j) + \partial_i p - \frac{1}{\text{Re}} \partial_{jj} u_i = 0, \quad i = 1, 2, 3, \quad (3)$$

where t denotes the time, u_i is the velocity in the Cartesian x_i direction, p is the pressure, and Re is the Reynolds number. Moreover, ∂_t and ∂_j are shorthand notations for $\partial/\partial t$ and $\partial/\partial x_j$, respectively. Finally, summation over repeated indices is implied.

In LES the large- and small-scale features of a flow solution are defined with reference to a low-pass filter. The solution is correspondingly decomposed as $u = \bar{u} + u'$ with large-scale component $\bar{u}$ and small scales u' . In LES one aims to arrive at an accurate prediction of the primary flow features contained in $\bar{u}$. Over the years a wide range of low-pass filters has been considered. Here, we will adopt integral filters. Following^{5,14} the nonuniform filtering to which we will restrict ourselves may be introduced in one spatial dimension as

$$\begin{aligned} \bar{u}(x) &= L[u](x) = \int_{-\infty}^{\infty} \frac{1}{\Delta(x)} G\left(\frac{y-x}{\Delta(x)}\right) u(y) dy \\ &= \int_{-\infty}^{\infty} G(s) u[x + \Delta(x)s] ds. \end{aligned} \quad (4)$$

The function G is referred to as the characteristic filter kernel which, for the sake of convenience, we assume does not depend explicitly on x . Obviously, an extension to characteristic filter kernels $G(x, s)$ is also possible but would only contribute to technical details in the presentation and will not be considered here. The filter operator L is required to be normalized, which corresponds to a filter kernel which should satisfy

$$\int_{-\infty}^{\infty} G(s) ds = 1, \quad (5)$$

and implies that constant solutions are invariant under L .

We will refer to a filter as “symmetric” if $G(s) = G(-s)$ and “skewed” or nonsymmetric otherwise. Skewness of a filter implies a particular “biasing” of the spatial averaging which, as a result, is no longer fully centered around the point x . Such a situation may readily arise in case the implementation of the filter is defined directly in terms of an underlying, nonuniform grid used for the simulations.⁶ In such cases, the skewness may explicitly depend on x . The specific

class of nonuniform filters considered in (4) corresponds to a constant skewness throughout the domain, which is sufficient for our purposes here.

We will consider general filters for which moments of fixed, but otherwise arbitrary order, defined as

$$M_k = \int_{-\infty}^{\infty} s^k G(s) ds, \quad k=0,1,2,\dots \quad (6)$$

exist. This excludes a popular filter such as the spectral cut-off filter but incorporates all compact support filters and the Gaussian filter as important examples. For symmetric filters all odd-numbered moments M_{2k+1} , $k=0,1,\dots$ are identically zero while skewness implies non-zero values for odd-numbered moments. In the sequel we will primarily consider an extension of the well-known symmetric top-hat filter. The use of this filter is numerically and analytically convenient, but our findings also hold for more general nonuniform filters.

For this top-hat filter we explicitly identify a skewness parameter γ and define the filter kernel in the following way:

$$G^{\text{th}}(s; \gamma) = \begin{cases} 1 & \text{if } -\frac{1}{2} + \gamma \leq s \leq \frac{1}{2} + \gamma \\ 0 & \text{otherwise.} \end{cases} \quad (7)$$

If we insert this filter kernel into (4) we find that filtered variables can be written as

$$\bar{u}(x) = L[u](x) = \int_{-(1/2)+\gamma}^{(1/2)+\gamma} u[x + \Delta(x)s] ds. \quad (8)$$

In this formulation of the top-hat filter, the “shift” γ is restricted to $\gamma \in [-\frac{1}{2}, \frac{1}{2}]$ so that the point x at least is in the support of the spatial filtering. The shift introduces skewness of the filter; in fact, we find $M_1 = \gamma$. The shift or skewness parameter γ is considered constant throughout this paper. In case $\gamma=0$ the familiar symmetric top-hat filter is reobtained.

An extension of the above one-dimensional filters to three dimensions can be obtained by simple composition, i.e., the three-dimensional filter $\mathcal{L}$ is defined as $\mathcal{L} = L_1 \circ L_2 \circ L_3$. Here, L_i corresponds to a filter associated with integration over the x_i direction which has a filter width $\Delta_i(\mathbf{x})$ and a shift γ_i . Note that with this definition of $\mathcal{L}$ the order in which the one-dimensional filter operations are applied is irrelevant. For the specific case of an extended top-hat filter the finite integration volume is always of “rectangular” shape, being the direct product of three intervals.

The filter width and its spatial nonuniformity can, in principle, be chosen independent of the grid on which the flow solution is obtained. As an example, in this paper DNS data that are available on a sufficiently fine uniform grid will be used to investigate properties of commutator errors and their explicit modeling. Separately, the filter-width nonuniformity can be specified in terms of scales that are a fraction of an (integral) length scale of the flow or a fraction of the size of the computational domain. In this case, the numerical implementation of the nonuniform spatial filtering should be sufficiently flexible to allow an accurate representation of the filter, despite the fact that the data are on a rather unrelated

computational grid. Here, we will adopt this setting solely to facilitate the detailed commutator-error analysis at a variety of filter-width nonuniformities. Of course, in situations where actual large-eddy simulations are performed, it is more sensible to include a direct connection between local grid spacing $h(\mathbf{x})$ and local filter width $\Delta(\mathbf{x})$. There is usually little sense in reducing the filter width in some region of the flow domain and not refining the computational grid locally as well. Specifically, one may connect grid and filter width, for example, such that Δ/h remains (approximately) constant throughout the domain.^{15–18}

The application of a nonuniform three-dimensional filter to the incompressible Navier-Stokes equations yields the complete, unclosed large-eddy equations. After some calculation the result may be expressed as

$$\partial_j \bar{u}_j = -C_j(u_j), \quad (9)$$

$$\begin{aligned} \partial_i \bar{u}_i + \partial_j (\bar{u}_i \bar{u}_j) + \partial_i \bar{p} - \frac{1}{\text{Re}} \partial_{jj} \bar{u}_i \\ = -\partial_j \tau_{ij} - C_j(u_i u_j) - C_i(p) + \frac{1}{\text{Re}} [C_j(\partial_j u_i) + \partial_j C_j(u_i)]. \end{aligned} \quad (10)$$

In (9) and (10) a number of closure terms have been identified on the right-hand side. In the nonuniformly filtered equations we observe that next to the divergence of the well-known turbulent stress tensor $\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$ several explicit commutator errors $C_j(f) = \overline{\partial_j f} - \partial_j \bar{f}$ arise as a result of the non-uniformity of the filter.

The filtered continuity equation (9) shows that nonuniform filtering gives rise to a smoothed velocity which is not solenoidal. This differs markedly from the unfiltered velocity or from the filtered velocity that arises when a traditional uniform convolution filter is used. In order to consistently incorporate this aspect of nonuniform LES, it is not sufficient to merely introduce subfilter models for the commutator errors and turbulent stresses, but also adaptations in the Poisson equation for the filtered pressure are required. Specifically, by taking the divergence of the filtered momentum equation (10) one may arrive at an expression for the Laplacian of the pressure $\partial_{ii} \bar{p}$. This extended Poisson equation contains a number of terms such as contributions due to the subfilter stresses $\partial_{ij} \tau_{ij}$ and the commutator errors, e.g., $\partial_i C_j(u_i u_j)$. However, apart from these terms, the divergence of the filtered velocity field also contributes to $\partial_{ii} \bar{p}$. In fact, we may write

$$\partial_{ij} (\bar{u}_i \bar{u}_j) = (\partial_i \bar{u}_j)(\partial_j \bar{u}_i) + (\partial_j \bar{u}_j)^2 + 2\bar{u}_i \partial_i (\partial_j \bar{u}_j). \quad (11)$$

This shows that apart from the usual term $(\partial_i \bar{u}_j)(\partial_j \bar{u}_i)$, additional terms arise which are directly associated with the divergence of the filtered velocity. Similarly, a term $\partial_i (\partial_j \bar{u}_j)$ arises in the extended Poisson equation. A self-consistent LES model can be arrived at in two steps. First, explicit subfilter models for the turbulent stresses and the commutator errors should be introduced in (9) and (10). Second, these subfilter models should also be incorporated into the extended Poisson equation for the filtered pressure. A more complete treatment of these issues is a subject of future re-

search and is beyond the scope of this paper. Instead, we will concentrate on the explicit modeling of the commutator errors themselves which, in turn, can be used as a part of the LES modeling and the extended Poisson equation.

In the sequel we will restrict ourselves to an analysis and explicit modeling of the commutator errors associated with the nonlinear convective flux, i.e., $C_j(u_i u_j) = \partial_j(u_i u_j) - \partial_j(\overline{u_i u_j})$. Central questions that we will address are related to the effects of filter nonuniformity on the resolved kinetic energy dynamics and how accurate this dynamics may be parametrized using explicit subfilter models for $C_j(u_i u_j)$ that reflect some of the Lagrangian character of these contributions.

Explicit modeling approaches for the commutator error have largely been left unexplored in the literature. Historically, the basic motivation for concentrating on modeling τ_{ij} while ignoring the commutator errors was provided by studying the scaling of commutator errors associated with the so-called higher-order filters. Specifically, higher-order filters have the property that $M_k = \delta_{k0}$ for $k=0, \dots, N-1$, where δ_{k0} denotes Kronecker's delta. An increase in the order of the filter was shown to imply a formal reduction in the magnitude of the commutator error. This would lead to negligible commutator errors in case N would become sufficiently large^{5,8,14,13,19} In detail, it may be shown that symmetric higher-order filters imply that the commutator error scales with $O(\Delta' \Delta^{N-1})$ (e.g., Ref. 13). However, this result by itself is incomplete, since the same higher-order filters imply that the turbulent stress $\partial_j \tau_{ij}$ shows similar scaling.^{7,8} In fact, the divergence of the turbulent stress tensor may be shown to scale with a dominant term of $O(\Delta' \Delta^{N-1})$ next to the more familiar scaling of order $O(\Delta^N)$. The latter contribution remains also in case the filter width is uniform while the other terms are specific to nonuniform filtering. The fact that both subfilter contributions $\partial_j \tau_{ij}$ and $C_j(u_i u_j)$ display the same dominant scaling for higher-order filters suggests that explicit commutator-error modeling approaches should be considered in regions of the flow domain where Δ' is significant. Conversely, if Δ' can be kept sufficiently bounded, the need for modeling nonuniformity of the filter may be effectively removed.

The actual magnitude of the individual closure terms was established in Ref. 7, using a direct numerical simulation database of turbulent mixing and a variety of filter-width nonuniformities. In this paper we concentrate specifically on the dynamics of the resolved kinetic energy associated with nonuniform filters. Moreover, we analyze the possibilities of explicit Lagrangian modeling of the commutator errors. We begin with energy dynamics in the following section.

III. RESOLVED KINETIC ENERGY DYNAMICS: CONSEQUENCES OF NONUNIFORM FILTERING FOR DISSIPATION AND DISPERSION

In this section we concentrate on the evolution equation for the resolved kinetic energy. First, we derive this equation in case the filter is spatially nonuniform (Sec. III A). Then, through a ‘‘Lagrangian’’ interpretation of the nonuniform filtering, the importance of skewness and of spatial variation of

the filter width is identified (Sec. III B). Finally, using a single-mode analysis, the explicit dissipative and dispersive contributions of the commutator error are illustrated. Combined with the Lagrangian interpretation of the commutator errors, this points toward a proposition for the explicit modeling of these effects (Sec. III C). The analysis of the kinetic energy dynamics in actual direct numerical simulation of developed turbulent mixing is postponed until Sec. IV while testing of the new commutator-error model will be considered in Sec. V.

A. Resolved kinetic energy equation

We consider a fixed flow domain $\Omega \subset \mathbb{R}^3$ and define the resolved kinetic energy E as

$$E(t) = \int_{\Omega} \frac{1}{2} \bar{u}_i \bar{u}_i d\mathbf{x}. \quad (12)$$

To characterize the various contributions to the evolution of E , we focus on two different quantities: (i) the local transport denoted by $\psi = -\partial_t(\frac{1}{2} \bar{u}_i \bar{u}_i)$ and (ii) the global dissipation rate $\varepsilon = -dE/dt$. Starting from the nonuniformly filtered momentum equation (10) one obtains after multiplication with $\bar{u}_i$ and summing over i ,

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

The total contribution arising from the nonlinear convective flux involves, next to the turbulent stress terms, the ‘‘basic mean’’ contribution $\bar{u}_i \partial_j (\bar{u}_i \bar{u}_j)$ and the ‘‘basic commutator-error’’ term $\bar{u}_i C_j(u_i u_j)$. Combined, these may be written in a convenient form as

$$\begin{aligned} \bar{u}_i \partial_j (\bar{u}_i \bar{u}_j) + \bar{u}_i C_j(u_i u_j) &= [\bar{u}_i \partial_j (\bar{u}_i \bar{u}_j) - \frac{1}{2} \bar{u}_i \bar{u}_i \partial_j \bar{u}_j] \\ &\quad + [\bar{u}_i C_j(u_i u_j) - \frac{1}{2} \bar{u}_i \bar{u}_i C_j(u_j)] \\ &= \frac{1}{2} \partial_j (\bar{u}_i \bar{u}_i \bar{u}_j) \\ &\quad + [\bar{u}_i C_j(u_i u_j) - \frac{1}{2} \bar{u}_i \bar{u}_i C_j(u_j)], \end{aligned} \quad (14)$$

where use was made of the nonuniformly filtered continuity equation $\partial_j \bar{u}_j = -C_j(u_j)$. This decomposition of the convective flux contribution incorporates the nonsolenoidal features of the nonuniformly filtered velocity field.^{4,7} Formally, it is analogous to the formulation that is commonly used for compressible flow; in the latter case $\psi = -\partial_t(\frac{1}{2} \bar{\rho} \bar{u}_i \bar{u}_i)$, where $\bar{u}_i = \bar{\rho} u_i / \bar{\rho}$ denotes the Favre-filtered velocity and $\bar{\rho}$ the density. In the compressible case the velocity is nonsolenoidal for physical reasons whereas here $\partial_j \bar{u}_j \neq 0$ due to nonuniformity of the filter. Following this convention, we may express ψ as

$$\psi = \psi_{\text{mean}} + \psi_p + \psi_{\text{visc}} + \psi_{\text{SFS}} + \psi_{\text{CE}}, \quad (15)$$

with individual contributions associated with the mean velocity field, pressure, viscous stresses, subfilter-scale stresses,

FIG. 1. Filtered (dashed) and unfiltered (solid) sine waves $f(x) = \sin(2\pi kx)$ with (a) $k=2$, (b) $k=6$, and (c) $k=12$ in the domain $[0, 1]$. The filter width $\Delta(x)$ (dotted) is nonuniform and specified as $\Delta(x)=1/5$ for $x < 1/2$ and $\Delta(x)=1/10$ for $x > 1/2$ with a short transition region around $x=1/2$.

and the “combined commutator error,” respectively. These contributions are defined explicitly as

$$\psi_{\text{mean}} = \bar{u}_i \left[\partial_j (\bar{u}_i \bar{u}_j) - \frac{1}{2} \bar{u}_i \partial_j \bar{u}_j \right] = \frac{1}{2} \partial_j (\bar{u}_i \bar{u}_i \bar{u}_j), \quad (16)$$

$$\psi_p = \bar{u}_i \partial_i \bar{p}, \quad (17)$$

$$\psi_{\text{visc}} = -\frac{1}{\text{Re}} \bar{u}_i \partial_{jj} \bar{u}_i, \quad (18)$$

$$\psi_{\text{SFS}} = \bar{u}_i \partial_j \tau_{ij}, \quad (19)$$

$$\psi_{\text{CE}} = \bar{u}_i \left[\mathcal{C}_j(u_i u_j) - \frac{1}{2} \bar{u}_i \mathcal{C}_j(u_j) \right]. \quad (20)$$

Regarding the transport of kinetic energy governed by the commutator error ψ_{CE} we will concentrate on the contributions associated with the convective flux. Hence, terms involving $\mathcal{C}_i(p)$ and $\text{Re}^{-1}[\mathcal{C}_j(\partial_j u_i) - \partial_j \mathcal{C}_j(u_i)]$ will no longer be included in the sequel.

Adding the filtered continuity equation as done in (14) typically involves only small additional terms in ψ_{CE} , but allows expressing the “combined mean contribution” as the divergence of $\bar{u}_i \bar{u}_i \bar{u}_j$. The corresponding global effect simplifies to a surface integral over the boundary of the flow domain, i.e.,

$$\varepsilon_{\text{mean}} = \frac{1}{2} \int_{\Omega} \partial_j (\bar{u}_i \bar{u}_i \bar{u}_j) d\mathbf{x} = \frac{1}{2} \int_{\partial\Omega} \bar{u}_i \bar{u}_i \bar{u}_j n_j dS, \quad (21)$$

where n_j denotes the outward pointing unit normal on the boundary $\partial\Omega$ of Ω . For various “popular” boundary conditions, e.g., periodic, free-slip, or no-slip conditions, the corresponding volume-integrated contribution to ε is therefore

zero.⁴ As a result the explicit contributions to the evolution of E therefore arise, from the pressure, viscous dissipation and the turbulent stresses, and the commutator errors. Hence, investigating ε provides a rather sensitive measure for the dynamical contributions from the various closure terms.

B. Interpretation of nonuniform filtering

In this section we first illustrate the application of a nonuniform filter in one spatial dimension. In particular, we concentrate on sine waves and focus on the local quality of resolution in relation to the wavenumber of the signal and the local filter width. Moreover, skewness is included and shown to affect the phase of the filtered signal. Subsequently, a Lagrangian interpretation of nonuniform filtering is formulated which characterizes the situation in three spatial dimensions. This provides a basis for explicit modeling of the corresponding commutator-error dynamics that will be considered momentarily.

The application of a filter effectively removes flow features that vary sufficiently rapidly on the scale of the local filter width. The appropriate parameter to quantify this for symmetric filters is $k\Delta(x)$, where k denotes the wavenumber of the signal. In Fig. 1 we illustrate the effect of abruptly varying Δ from one value in the first half of the domain to another value in the second half. For illustration purposes, if the sine wave is reduced in amplitude by about 50% or more, we will refer to it as “subfilter” while it is considered “resolved” otherwise. For the nonuniform top-hat filter considered in this example this rough identification implies that if $k\Delta(x) \lesssim 1/2$ then the corresponding signal may be considered locally resolved. Specifically in this example, we notice that, e.g., the $k=2$ mode can be considered resolved through-

FIG. 2. Filtered (dashed) and unfiltered (solid) sine waves $f(x)=\sin(2\pi kx)$ with (a) $k=1$ and (b) $k=2$ in the domain $[0, 1]$. The filter is maximally skewed with $\gamma=\frac{1}{2}$ and the filter width $\Delta(x)$ (dotted) is nonuniform and specified as $\Delta(x)=1/5$ for $x < 1/2$ and $\Delta(x)=1/10$ for $x > 1/2$ with a short transition region around $x=1/2$.

out the domain while the mode at $k=12$ clearly is subfilter everywhere. The interesting modes are in between, e.g., at $k=6$, which may be considered subfilter in part of the domain and resolved in other parts of the domain.

We may associate the actual effect of a nonuniform filter with the transition from resolved to subfilter for specific modes. Before this transition from resolved to subfilter is used to clarify the dynamic behavior of the commutator error $\mathcal{C}_j$, the particular effect due to filter skewness is illustrated.

1. Effect of skewness

The effect of skewness of a filter can most readily be illustrated by applying the skewed top-hat filter introduced in (8) to a single sine wave $u=\sin(2\pi kx)$. Direct evaluation of the filter yields the filtered velocity given by

$$\bar{u}(x) = A(k\Delta) \sin\{2\pi k[x + \Delta(x)\gamma]\}, \quad (22)$$

where the damping factor A depends on $k\Delta$ as

$$A(k\Delta) = \frac{\sin(\pi k\Delta)}{\pi k\Delta}. \quad (23)$$

We observe that the amplitude reduction for the skewed top-hat filter is not influenced by explicit skewness. Instead, the effect of explicit filter skewness (i.e., $\gamma \neq 0$) is clearly recognized by a local phase shift. This implies that the filtered signal is either lagging or leading the original wave depending on $\Delta\gamma$. In Fig. 2 we illustrate the case in which $\gamma=\frac{1}{2}$. This clearly illustrates that the phase shift by which the filtered wave lags behind the unfiltered signal is reduced from $\gamma/5$ to $\gamma/10$ when passing the nonuniformity from left to right. Hence, the reduction of filter width in the direction of the wave propagation implies next to an increase in amplitude of the resolved wave also a reduction of phase shift when $\gamma \neq 0$. This illustrates clearly both dispersive and dissipative effects arising from nonuniform, skewed filtering, which was already recognized by Vasilyev *et al.*¹³ and Geurts *et al.*⁶

We will next extend the interpretation of commutator errors to three spatial dimensions.

2. Lagrangian interpretation of commutator errors

In Fig. 3 a nonuniform grid is sketched which can resolve different ranges of wavenumbers depending on the location in the grid. If we consider a particular flow path as indicated then for $x < x_a$ all scales up to k_{coarse} may be resolved while for $x_a < x < x_b$ the filter width is decreased such that scales in the range $[k_{\text{coarse}}, k_{\text{fine}})$ also become available as resolved scales.

The local effect corresponding to a decrease of the filter width can be interpreted as an effective production of resolved kinetic energy. Similarly, if the nonuniform filter width is increased, this should result in a decrease of resolved kinetic energy, e.g., contributing to an effective dissipation. Correspondingly, the commutator errors can be associated with the apparent local creation/destruction of turbulent flow scales if the filter width is decreased/increased along a flow path. Hence, the contributions arising from the commutator error are directly linked to the magnitude and sign of changes in the filter width in the direction of the local flow path. Large variations in Δ do not necessarily imply

FIG. 3. An illustration of filter-width variations which induce commutator errors that represent the apparent creation and destruction of scales associated with variations in the local resolution of the flow. An increased local resolution in the direction of the flow, corresponds to an apparent creation of small-scale flow structures while a reduced resolution may be associated with the annihilation of the corresponding flow structures.

large commutator-error contributions in an actual simulation; only if these changes occur in the direction of the local flow, can commutator-error dynamics become essential. This suggests a direct modeling in terms of the material derivative of Δ which contains the central contribution $u_j \partial_j \Delta$, expressing exactly this observation.

The proposed Lagrangian modeling emphasizes a specific directional dependence of the commutator error. This can be further illustrated and motivated by considering a flow $\mathbf{u} = [u_1(x_2), u_2^{(0)}, u_3^{(0)}]$, at constant pressure p . Here, $u_2^{(0)}, u_3^{(0)}$ are (possibly nonzero) constant velocities in the x_2 and x_3 directions. This flow is slightly more general than a strict unidirectional flow. We introduce nonuniform filtering using a normalized product filter $\mathcal{L} = L_1 \circ L_2 \circ L_3$. We assume L_1 and L_3 to be convolution filters with constant filter widths Δ_1 and Δ_3 and only L_2 is a nonuniform filter with filter width $\Delta_2(x_2)$. This setting implies nonzero commutator errors corresponding to ∂_2 only, i.e., $\overline{\partial_1 f} = \partial_1 \bar{f}$, $\overline{\partial_2 f} \neq \partial_2 \bar{f}$ and $\overline{\partial_3 f} = \partial_3 \bar{f}$ for any field f .

For this flow configuration we next evaluate all terms that arise in the filtered equations (9) and (10). First, one may readily verify that $C_j(u_j) = 0$. Next, with respect to the momentum equations, the constant pressure implies that all pressure contributions are zero. One may verify that actually all fluxes in the momentum equations for the x_2 and x_3 directions are zero. The only nontrivial equation is the momentum equation in the x_1 direction for which we find

$$\partial_t \bar{u}_1 + u_2^{(0)} \partial_2 \bar{u}_1 - \frac{1}{\text{Re}} \partial_{22} \bar{u}_1 = -u_2^{(0)} C_2(u_1) + \frac{1}{\text{Re}} [C_2(\partial_2 u_1) + \partial_2 C_2(u_1)]. \quad (24)$$

Since $\partial_t \bar{u}_2 = \partial_t \bar{u}_3 = 0$ in this case, we observe that the initial structure of the flow is maintained. The only commutator errors of interest are $C_2(u_1 u_2) = u_2^{(0)} C_2(u_1)$ and a small contribution due to the viscous flux commutator error. In case of strict unidirectional flow the normal velocity component $u_2^{(0)} = 0$ and no filter-width variations are encountered along a flow path. In this case the commutator error $C_2(u_1 u_2)$ has no contribution to the evolution of the flow. Only when $u_2^{(0)} \neq 0$ a nonzero commutator error arises, which corresponds directly to the nonzero filter-width variations along a flow path. The proposed Lagrangian interpretation and modeling in terms of the material derivative of the filter width is fully consistent with this situation.

C. Single-mode analysis of commutator-error dynamics

In this section we will consider the effect of nonuniform, skewed filtering and specify in some detail the commutator error associated with individual Fourier modes in a solution. This will further specify the connection with the material derivative of the filter width, argued in the preceding section.

In the single-mode analysis of the commutator error we assume that $u = \exp(ikx)$. Application of the skewed top-hat filter yields

$$\bar{u} = A\left(\frac{k\Delta}{2}\right) e^{ik(x+\Delta\gamma)} = A\left(\frac{k\Delta}{2}\right) u(x + \Delta\gamma) \quad (25)$$

with damping function A given by (23). The modified wavenumber k' , as introduced by Ghosal and Moin,⁵ may be used in quantifying the commutator error. Specifically, k' is defined through $\partial_x \bar{u} = ik' \bar{u}$. For symmetric filters the commutator error may be shown to be mainly diffusive.⁵ In the following, we will derive the modified wavenumber corresponding to skewed filters and show that both diffusive and dispersive contributions arise in that case.¹³

From (25) one can easily derive that

$$\begin{aligned} \partial_x \bar{u} &= \partial_x \left[A\left(\frac{k\Delta}{2}\right) u(x + \Delta\gamma) \right] \\ &= F\left(\frac{k\Delta}{2}\right) \frac{k\Delta'}{2} \bar{u} + i(1 + \Delta'\gamma) k \bar{u}, \end{aligned} \quad (26)$$

where, for the skewed top-hat filter, the function F is given by

$$F\left(\frac{k\Delta}{2}\right) = -\left[\frac{2}{k\Delta} - \cot\left(\frac{k\Delta}{2}\right) \right]. \quad (27)$$

Correspondingly, using the definition of the modified wavenumber k' , we find

$$k' = -iF\left(\frac{k\Delta}{2}\right) \frac{k\Delta'}{2} + (1 + \Delta'\gamma)k. \quad (28)$$

This expression of the modified wavenumber k' contains the expression found in Ref. 5, as well as a dispersive contribution $\gamma\Delta'$ which is encountered for nonzero skewness $\gamma \neq 0$.¹³ We will next derive the single-mode expression for $\bar{u} C_x(u^2)$ and make the connection with the material derivative of Δ more explicitly. Extended to three dimensions $\bar{u} C_x(u^2)$ is closely related to $\bar{u}_i C_j(u_i u_j)$ which again is the main contributor to the transport of resolved kinetic energy by the commutator error ψ_{CE} .

The single-mode expression for the commutator error of the convective flux $C_x(u^2)$ is given by

$$\begin{aligned} C_x(u^2) &= \overline{\partial_x e^{2ikx}} - \partial_x \overline{e^{2ikx}} = \overline{\partial_x e^{2ikx}} - \partial_x [A(k\Delta) e^{2ik(x+\Delta\gamma)}] \\ &= 2ike^{2ikx} - 2ik(1 + \Delta'\gamma) e^{i2kx} + F(k\Delta) e^{2ik(x+\Delta\gamma)}. \end{aligned} \quad (29)$$

This may be rewritten as

$$C_x(u^2) = -\Delta' \gamma \overline{\partial_x u^2} + \frac{\Delta'}{\Delta} F(k\Delta) \overline{u^2}, \quad (30)$$

such that $\bar{u} C_x(u^2)$ is given by

$$\begin{aligned} \bar{u} C_x(u^2) &= \bar{u} \left(-\gamma \overline{\partial_x u^2} + F(k\Delta) \frac{\overline{u^2}}{\Delta} \right) \Delta' \\ &= \left(-\gamma \overline{\partial_x u^2} + F(k\Delta) \frac{\overline{u^2}}{\Delta} \right) \frac{D\Delta}{Dt}. \end{aligned} \quad (31)$$

In (31) we recognize two distinct contributions which we will discuss next.

The interpretation of the commutator error given in the preceding section suggests to parametrize ψ_{CE} in terms of the material derivative of $\Delta_j(\mathbf{x})$ along a flow path, i.e., $D_t \Delta_j = \partial_t \Delta_j + \bar{u}_k \partial_k \Delta_j = \bar{u}_k \partial_k \Delta_j$ in case Δ_j does not explicitly depend on time t . By defining ℓ and T as characteristic length and time scales, one can readily verify that $D_t \Delta_j$ has dimension ℓT^{-1} , whereas the dimension of ψ_{CE} equals $(\ell T^{-1})^3 \ell^{-1}$. Accounting for the proper physical dimension the following specific parametrization for ψ_{CE} is evident:

$$\psi_{\text{CE}} \sim \frac{|\bar{\mathbf{u}}|^2}{\Delta_j} \bar{u}_k \partial_k \Delta_j \equiv \xi_0, \quad (32)$$

where $|\bar{\mathbf{u}}|^2 = \bar{u}_i \bar{u}_i$. The front factor $F(k\Delta)$ in (31) further quantifies this contribution and shows that this term is small in case $k\Delta \ll 1$, as is to be expected for all subfilter contributions. In the sequel, we will use the notation ξ_0 to represent this part of the commutator error. Expression (32) includes the material derivative of $\ln(\Delta_j)$ which is a measure of the relevance of the commutator error relative to the turbulent stresses.⁸ Inspection of (31) indicates that skewness provides an additional contribution $\sim \partial_x u^2 D_t \Delta$ which has a similar interpretation as a ratio between the square of a characteristic velocity and a length scale multiplied by the material derivative of the filter width.

An explicit parametrization for the commutator-error contribution can be obtained by observing that $\bar{u}^2/\Delta = \bar{u}^2/\Delta + O(\Delta)$ and $\partial_x \bar{u}^2 = \partial_x \bar{u}^2 + O(\Delta')$ when $\gamma \neq 0$. Guided by (31) the following model for the transport of resolved kinetic energy is proposed:

$$\psi_{\text{CE}} \approx \xi \equiv c_0 \xi_0 - c_1 \xi_1, \quad (33)$$

with c_0 and c_1 constants to which we return momentarily, and ξ_1 given by

$$\xi_1 = \gamma_j \frac{\partial |\bar{\mathbf{u}}|^2}{\partial x_j} \frac{D \Delta_j}{Dt}. \quad (34)$$

In the following section we will consider the kinetic energy dynamics associated with general nonuniform, skewed filters, applied to turbulent mixing and use statistical analysis to verify (33).

IV. COMMUTATOR-ERROR ENERGY DYNAMICS IN TURBULENT MIXING

In this section we will first introduce the temporal mixing layer which provides the turbulent flow data used in the analysis of the kinetic energy dynamics. Moreover, we will specify the nonuniformities in the filter and describe the statistical evaluation method with which we will quantify the agreement between the actual ψ_{CE} and its explicit Lagrangian modeling hypothesis (33). This will be collected in Sec. IV A. Subsequently, we will present results for the kinetic energy dynamics obtained by evaluating the nonuniformly filtered direct numerical simulation database in Sec. IV B. The consequences of the Lagrangian modeling hypothesis for the direct representation of the commutator errors as arise on flux level in the momentum equations form a separate issue that will be presented in Sec. V.

A. Temporal mixing layer and statistical evaluation method

In order to assess the Lagrangian modeling hypothesis for the commutator error energy dissipation rate ψ_{CE} we will use turbulent flow in a temporal mixing layer at Reynolds number $\text{Re}=50$. The mixing layer flow displays a strong transition to small-scale turbulence and is well suited for studying the accuracy and implications of (33). By correlating ψ_{CE} with the proposed model, we may illustrate the quality of the Lagrangian hypothesis, both for symmetric as well as for skewed filters.

The governing Navier-Stokes equations are solved using fourth-order accurate finite volume discretization and explicit Runge-Kutta time stepping. A cubic geometry of side ℓ is adopted in which ℓ is set equal to four times the wavelength of the most unstable mode according to the linear stability theory. Periodic boundary conditions are imposed in the streamwise (x_1) and spanwise (x_3) directions, while in the normal (x_2) direction the boundaries are free-slip walls. We use a resolution of 192^3 grid cells. 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 this mean profile are two- and three-dimensional perturbation modes obtained from the linear stability theory. For further details we refer to Vreman *et al.*⁴ In Fig. 4 we illustrate the evolution of the temporal mixing layer, displaying two separate pairings, first from four spanwise rollers to two and subsequently from two to one roller. During this process the flow becomes strongly three-dimensional and a complicated flow arises with many small-scale features and various regions with positive and negative spanwise vorticities.

The evaluation of the different contributions to the kinetic energy dynamics is done with respect to filter widths that are constant in the homogeneous x_1 and x_3 directions. Instead, the filter width associated with the x_2 direction is nonuniform and clustered near the centerline of the mixing layer, since this region displays strong gradients that would require a reduced filter width in order to enhance their spatial resolution. Variations in Δ_2 are chosen to be Gaussian and in total we adopt

$$\Delta_1 = \Delta_3 = \Delta_r, \quad \Delta_2(x_2) = \Delta_r(1 - \alpha e^{-(\beta x_2/\ell)^2}). \quad (35)$$

The reference filter width Δ_r is taken equal to $\ell/16$. This provides a test case for large-eddy simulation in which the subfilter contributions are significant.⁴ In the definition of the nonuniform filter width $\Delta_2(x_2)$ the parameter α controls the “depth” of the filter-width modulation, while β controls its width. The minimal filter width $\Delta_{\min} = \Delta_r(1 - \alpha)$ and in this paper we will use $\alpha=3/4$. In Fig. 4 different realizations of this nonuniform filter width have been superimposed on snapshots of the flow. The filtered quantities needed in the evaluation of the kinetic energy dynamics are obtained using the composite trapezoidal rule applied to the top-hat filter. In case end points of the integration domain are in between two grid points, linear interpolation is used to approximate the values at the end points. The required spatial derivatives are

FIG. 4. Contour plots of the spanwise vorticity of the developing mixing layer at (a) $t=20.0$, (b) $t=50.0$, and (c) $t=80.0$. Nonuniform filter widths as defined in (35) with $\alpha=3/4$ and $\beta=5$ (dashed), $\beta=10$ (solid) and $\beta=30$ (dotted) are superimposed on these plots.

approximated using second-order accurate central finite differencing with grid spacing $\Delta_r/4$.

To test the kinetic energy parametrization expressed in (33) we will interpret ψ_{CE} and ξ as stochastic variables and

quantify their main features using a statistical analysis. Since the filter is non-uniform in the x_2 direction only, the model ξ reduces to

$$\xi = \left(c_0 \frac{\bar{u}_i \bar{u}_i}{\Delta_2} - c_1 \gamma_2 \partial_2 \bar{u}_i \bar{u}_i \right) \bar{u}_2 \Delta_2'. \quad (36)$$

In order to assess the quality of the Lagrangian model we will focus on the correlation between ψ_{CE} and ξ . Moreover, we determine the pair distribution function (PDF) $P(\xi, \psi_{CE})$ using a standard binning procedure for these two quantities, which expresses their connections in further detail. We will consider the results of this evaluation both for symmetric as well as for skewed filters.

B. Correlation and PDF of energy dynamics model

In this section we test the modeling of ψ_{CE} and distinguish between symmetric and skewed filters. First, we turn to symmetric filters in which case ξ reduces to ξ_0 . Subsequently, we will extend the testing to skewed filters and focus on the effectiveness of the proposed additional contribution ξ_1 .

1. Symmetric filters

The correlation between ψ_{CE} and ξ for symmetric filters at different filter-width nonuniformities was studied. Quite low correlation was observed in the initial, laminar, and transitional stages in cases where the filter width is only mildly nonuniform but over quite an extended region, e.g., corresponding to $\beta=5$ or $\beta=10$. This low correlation is associated with the fact that either $\Delta_2' \approx 0$ in the region around the centerline, or, initially, $\bar{u}_2 \approx 0$ in large parts of the domain [see Fig. 4(a)]. Consequently, the model in (36) is virtually zero in these phases of the flow development. However, once the mixing layer has evolved away from the centerline into the parts of the domain where Δ_2' is significant, a comparably high correlation of about 0.6 is observed.

More detail regarding the quality of (33) can be inferred from the PDF $P(\xi, \psi_{CE})$. For the calculation of the PDF a binning procedure²⁰ has been used in terms of the quantities ξ^* and ψ_{CE}^* which are given by ξ and ψ_{CE} normalized by their root-mean-square values, i.e.,

$$\xi^* = \frac{\xi}{\langle \xi^2 \rangle^{1/2}}, \quad \psi_{CE}^* = \frac{\psi_{CE}}{\langle \psi_{CE}^2 \rangle^{1/2}}. \quad (37)$$

In Fig. 5 we observe that the PDFs are localized around the origin, since either $\bar{u}_2$ or Δ_2' is small in large parts of the domain; observe the contour levels used in the figure. More importantly, we observe that contours of the PDFs are mainly located in the first and third quadrants, which underlines the quality of the hypothesis formulated in (33). The predominance of contour lines in the first and third quadrants indicates that whenever $|\psi_{CE}^*|$ is large, so is $|\xi^*|$, and that in addition the signs correlate very well. These aspects are certainly required in order for the modeling hypothesis to be accurate.

The PDFs can be used to obtain one-dimensional conditional averages which further quantify the effectiveness of the model ξ . As an example, it is expected that “events” in

FIG. 5. The PDF $P(\xi, \psi_{CE})$ for the flow at $t=60$, with nonuniform filter widths corresponding to $\alpha=3/4$ and (a) $\beta=5$, (b) $\beta=10$, and (c) $\beta=30$.

FIG. 6. The stochastic variables (a) $\Psi^+(\xi)$ and (b) $\mathcal{E}(\xi)$ in case $\alpha=3/4$, $\beta=10$, and $t=40$ (dotted), $t=60$ (solid), and $t=80$ (dashed).

which $\psi_{CE}^* > 0$ will correspond closely with locations where $\xi > 0$ and vice versa. This relation may be illustrated by considering what we will refer to as the positivity correlation:

$$\Psi^+(a) = \langle \psi_{CE} > 0 | \xi = a \rangle. \quad (38)$$

The function Ψ^+ denotes the expectation that the dissipation is positive given the value of ξ . It is expected that $\Psi^+(a) \rightarrow 1$ for $a > 0$ and $\Psi^+(a) \rightarrow 0$ for $a < 0$, i.e., the commutator-error dissipation is positive whenever the modeled term is and vice versa. In fact, there should be a sharp “crossover” from $\Psi^+ \approx 0$ to $\Psi^+ \approx 1$ as a changes sign, to indicate that the Lagrangian modeling hypothesis is accurate. Closely related is the conditional expectation of ψ_{CE} as a function of a ,

$$\mathcal{E}(a) = \langle \psi_{CE}^* | \xi = a \rangle. \quad (39)$$

Close correlation of ψ_{CE} and ξ would imply an approximately linear dependence of $\mathcal{E}$ as function of a .

In Fig. 6 we plotted Ψ^+ and $\mathcal{E}$ for the characteristic case $\alpha=3/4$ and $\beta=10$ at various stages in the development of the flow. In Fig. 6(a) the expected behavior of Ψ^+ is indeed

FIG. 7. The positivity correlation $\Psi^+(\xi)$ between ψ_{CE} and the dissipative model ξ_0 at $t=60.0$ in case $\alpha=3/4$ and $\beta=10$ for the symmetric case $\gamma=0$ (solid) and various values of the skewness: $\gamma=\frac{1}{10}$ (dash-dot), $\gamma=\frac{1}{4}$ (dotted), and $\gamma=\frac{1}{2}$ (dashed).

observed, including the sharp transition around $\xi^*=0$. In Fig. 6(b) an almost linear relation between $\mathcal{E}$ and ξ is observed, which further establishes the quality of the new parametrization for symmetric filters.

2. Skewed filters

Next, we turn to skewed filtering in the definition of the commutator errors. First, we establish that the originally proposed parametrization (32) is no longer adequate for nonzero skewness and that the dispersive part ξ_1 needs to be included. Next, we will study the effect of varying the relative importance of the dissipative (ξ_0) and the dispersive (ξ_1) contributions in the Lagrangian model, for various values of the filter skewness.

In Fig. 7 we display Ψ^+ for several values of the skewness parameter γ and a characteristic turbulent field obtained at $t=60.0$. In this figure the sharp crossover around $\xi=0$ is still present, but the size of the “jump” becomes smaller as the skewness increases. The desired behavior in which that $\Psi^+(\xi) \rightarrow 0$ for $\xi < 0$ and $\Psi^+(\xi) \rightarrow 1$ for $\xi > 0$ is not so clear for $\gamma \neq 0$. For example, for $\gamma=\frac{1}{2}$, $\Psi^+(\xi)$ tends to 0.45 for $\xi < 0$ and to 0.65 for $\xi > 0$. The correlation coefficient was found to drop to ≈ 0.15 in cases of maximal skewness $\gamma = \pm \frac{1}{2}$.

The failure of ξ_0 to cover all aspects of ψ_{CE} suggests the need to include the explicit dispersive contributions due to ξ_1 in case the filter is skewed. Hence, we next extend the testing to the full parametrization (33) where $\xi=c_0\xi_0-c_1\xi_1$ with parameters c_0 and c_1 . In Fig. 8 we show Ψ^+ for various values of c_1/c_0 at skewness $\gamma=\frac{1}{2}$. The expected behavior of Ψ^+ is similarly recovered by incorporating ξ_1 into the model, and compares well with that obtained in the symmetric filter case. As $c_1/c_0=30$ the correlation coefficients are ≈ 0.55 which is comparable to the values found in the symmetric case.

FIG. 8. The positivity correlation $\Psi^+(\xi)$ between ψ_{CE} and the full Lagrangian model $\xi=c_0\xi_0-c_1\xi_1$ in case the filter width is given by $\alpha=3/4$ and $\beta=10.0$ at $t=60.0$ and skewness $\gamma=\frac{1}{2}$ with various values of the ratio c_1/c_0 , $c_1/c_0=0$ (dashed), $c_1/c_0=5$ (dash-dot), $c_1/c_0=30$ (dotted), and $c_1/c_0=\infty$ (dash-dot-dot). For comparison also the symmetric result is given in both figures (solid).

The dependence of correlation and Ψ^+ on the ratio c_1/c_0 naturally leads to the question what ratio is optimal. In Fig. 9(a) the correlation is shown as a function of c_1/c_0 at various moments in time for $\gamma=\frac{1}{2}$. We notice that the correlation has a peak near $c_1/c_0 \approx 13$. Moreover, this “optimal” value for c_1/c_0 is quite independent of the skewness parameter γ as shown in Fig. 9(b). The limiting cases corresponding to $c_1/c_0=0$ or $c_1/c_0=\infty$, i.e., when c_1 or c_0 is zero, correspond to the individual correlation of the diffusive ξ_0 and the dispersive part ξ_1 , respectively. Consequently these limiting cases indicate whether for a given skewness either dissipation or dispersion is dominant. Clearly, when $\gamma \approx 0$ and the behavior of the commutator error is diffusive a high correlation is observed when $c_1=0$, while the correlation is zero when $c_0=0$. If the skewness increases then dispersion becomes more and more important. Moreover, already for $\gamma=\frac{1}{4}$ the individual correlation for the dispersive part ξ_1 is higher than that for the diffusive part ξ_0 and the dynamical behavior of the commutator error is dominated by dispersion rather than diffusion.

More global information can be gathered from Fig. 10. In this figure contours of the correlation between ψ_{CE} and ξ are shown as a function of c_1/c_0 as well as the skewness γ . The graphs shown in Fig. 9(b) are horizontal intersections of Fig. 10 for a given skewness γ . As can be seen in this figure in a small band around $\gamma=0$ dispersive effects are absent as the highest correlation is observed for $c_1=0$. For $|\gamma| > \frac{1}{10}$ the relative importance of dispersion increases considerably with increasing skewness. In this regime where dispersive effects are important the tendency of the correlation to peak at a constant value of the ratio c_1/c_0 is also observed. This tendency was already observed in Fig. 9(b) and is in Fig. 10 depicted by the ∇ symbols. For a given skewness these symbols indicate the peak correlation. For this particular snapshot of the flow and typical filter width layout the location of

FIG. 9. The correlation between ψ_{CE} and ξ as a function of the ratio between c_1 and c_0 . (a) $\gamma = \frac{1}{2}$ at various moments in time, $t=40.0$ (dashed), $t=50.0$ (dotted), $t=60.0$ (solid), and $t=70.0$ (dash-dot). (b) $t=60.0$ and $\gamma = \frac{1}{2}$ (solid), $\gamma = \frac{1}{4}$ (dashed), $\gamma = \frac{1}{10}$ (dotted), $\gamma = \frac{1}{20}$ (dash-dot), $\gamma = \frac{1}{100}$ (dash-dot-dot), and $\gamma = \frac{1}{1000}$ (long dash).

the maximum correlation is observed when $c_1/c_0 \approx 13$. Other snapshots and other filter-width layouts indicate that the optimal ratio should be somewhere between 10 and 30.

In this section we have shown that the parametrization (33) can capture the dominant dissipative and dispersive aspects of the local transport of resolved kinetic energy arising from the commutator error. The results generally show high correlation between ψ_{CE} and ξ for both symmetric and skewed filters. In the following section we will hence consider the corresponding subfilter model for the commutator-error fluxes $C_j(u_i u_j)$ as arise directly in the momentum equation. Moreover, we will compare the resulting model with other explicit CE models arising from general similarity assumptions.

V. ASSESSMENT OF LAGRANGIAN MODEL FOR THE COMMUTATOR ERROR

In this section we introduce and test a new explicit model for the commutator error, based on the Lagrangian

FIG. 10. Contour plot of the correlation between ψ_{CE} and ξ as a function of the ratio between c_1 and c_0 and the skewness γ when $t=60$, $\alpha=0.75$, and $\beta=10$. The contours increment is 0.02. The ∇ symbols indicate the location of maximum correlation for a given skewness.

model (33) for the local transport of kinetic energy. We first describe the parametrization for $C_j(u_i u_j)$ and subsequently compare this new model with two similarity-type CE models (see also Ref. 7).

The flux associated with the commutator error in the momentum equations is central to the development of large-eddy simulation in complex domains. These terms require explicit modeling in case variations of the filter width in the direction of the local flow are sufficiently strong. In line with the Lagrangian model (33) and the physical dimension of the commutator-error flux the following CE model is proposed for the case Δ_j does not depend explicitly on t :

$$C_i^{\text{Lag}} = \left\{ d_0 \frac{\bar{u}_i}{\Delta_j} - d_1 \gamma_j \partial_j \bar{u}_i \right\} D_i \Delta_j; \quad D_i \Delta_j = \bar{u}_k \partial_k \Delta_j, \quad (40)$$

with d_0 and d_1 appropriate (dynamic) constants and γ_j the skewness parameter for the x_j direction. This model represents the Lagrangian interpretation discussed above in Sec. III B and includes separate contributions associated with skewness of the filter.

The Lagrangian CE model (40) will be compared with two other commutator-error models that are based on the similarity assumption and were first put forward in Ref. 8. The first model that will be considered is the similarity CE model. This model extends Bardina's similarity assumption for the turbulent stress tensor²¹ to also cover commutator errors on flux level. Following the definition of the commutator error, and applying this to the available resolved velocity field, we arrive at

$$C_i^{\text{sim}} = \partial_j (\bar{u}_i \bar{u}_j) - \partial_j (\bar{u}_i \bar{u}_j). \quad (41)$$

The second model that will be considered is the gradient formulation of (41) in line with the original Clark model for the turbulent stress tensor.²² This model is computationally less expensive than the similarity model, since it does not require any additional filtering operations. It is given by

FIG. 11. The L_2 norm of $C_j(u_i u_j)$ and C_1^{mod} as a function of the normal x_2 direction for the symmetric case: exact (solid), similarity (dotted), gradient (dashed), Lag with $d_0=0.05$ (dash-dot).

$$C_i^{\text{gradient}} = -\{M_{k1}(\partial_j \Delta_k) \partial_k (\bar{u}_i \bar{u}_j) + M_{k2} \Delta_k (\partial_j \Delta_k) \partial_{kk} (\bar{u}_i \bar{u}_j)\}, \quad (42)$$

where M_{k1} and M_{k2} are the first and second moments of the filter in the k th direction. For a symmetric filter associated with the k th direction, $M_{k1} \equiv 0$. Similar to the original gradient model for the turbulent stress tensor, this model may be motivated using Taylor expansions of the filter operator in the mathematical limit of very small filter width and applied to smooth velocity fields.

We will assess the quality of the different models by focusing on the correlation with the exact commutator error as obtained from the DNS data and by comparing profiles of the corresponding fluxes for the different CE models. We first turn to symmetric filters and consider skewed filtering afterwards.

A. Symmetric filters

The correlation between the exact and the various modeled commutator-error representations reveals that the similarity CE model shows a very high correlation of 0.94, while the gradient models shows a correlation of 0.77. The Lagrangian CE model performs rather poorly as far as correlation is concerned, with a correlation around 0.44. The high correlation of the similarity-type models is reminiscent of the situation that arises when modeling the turbulent stress tensor, especially at relatively modest filter widths.

The L_2 norm of the commutator-error flux over planes at constant x_2 provides a clear profile with which the actual dynamic contribution of these terms and their proposed models can directly be compared. For any field $f(\mathbf{x})$ this L_2 norm is given by

$$L_2(f)(x_2) = \left(\frac{1}{\ell_1 \ell_3} \iint f^2(\mathbf{x}) dx_1 dx_3 \right)^{1/2}. \quad (43)$$

In Fig. 11 the resulting L_2 profiles for $C_j(u_i u_j)$ and C_1^{mod} are shown. The similarity and gradient CE model tend to, re-

FIG. 12. The L_2 norm of $C_j(u_i u_j)$ as a function of the normal x_2 direction as predicted by the commutator-error models with skewness given by (a) $\gamma = 1/4$ and (b) $\gamma = 1/2$ and the filter width by $\alpha=0.75$ and $\beta=10$: exact (solid), similarity (dotted), Clark (dashed), Lagrangian model with $d_0=0.05$ and $d_1=0.8$ (dash-dot), and Lagrangian model with $d_0=0.05$ and $d_1=1.0$ (dash-dotted).

spectively, underpredict or overpredict the L_2 profile, but their shape is generally in good agreement with the exact L_2 profile of $C_j(u_i u_j)$. The location of the maxima above and below the centerline are predicted well with these models. The Lagrangian model tends to position these maxima slightly too close to the centerline. By selecting, e.g., $d_0=0.05$ the magnitude of these extrema may be predicted accurately using the Lagrangian model. Since the commutator error also satisfies the Germano identity, there is a natural option to determine the model coefficients using the dynamic procedure.

B. Skewed filters

For skewed filters the correlation of the similarity and gradient model drops to 0.65 and 0.58, respectively, as $\gamma = \frac{1}{2}$. The correlation of the Lagrangian model at this maximum skewness is about 0.61 as $d_1/d_0=20$. In Fig. 12 the L_2 profile is shown for the various models in case the skewness parameter $\gamma=1/2$. For the Lagrangian model the realizations

are shown with $d_0=0.05$ and d_1 either 0.8 or 1.0, corresponding to $d_1/d_0 \approx 20$. The Lagrangian model corresponds much closer to the actual commutator error in the skewed case, producing approximately similar agreement as the other two models. For example, the peaks above and below the centerline are predicted well by the Lagrangian model in this case. In actual simulations of turbulent mixing on strongly nonuniform grids the dynamic consequences of the Lagrangian model and the two similarity models will need to be assessed in order to further substantiate these observations and to quantify the relevance of the dissipative and dispersive properties of the commutator errors. This is a subject of ongoing research.

VI. CONCLUDING REMARKS

In this paper we studied the effects of the commutator error on the dynamics of the resolved kinetic energy and in relation to the momentum equation. It was argued that the commutator error can be associated with the apparent local creation or destruction of resolved turbulent flow scales. In turn, this leads to a local increase or decrease in resolved kinetic energy, depending on the variations in the filter width Δ .

In the Lagrangian interpretation, the effect of a nonuniform filter width on the resolved kinetic energy can be captured in terms of the material derivative of the filter width $D_t \Delta = \partial_t \Delta + \bar{u}_i \partial_i \Delta$. Correspondingly, the local transport of kinetic energy by the commutator error, ψ_{CE} , was modeled by

$$\psi_{CE} \approx \xi = \left(c_0 \frac{|\mathbf{u}|^2}{\Delta_j} - c_1 \gamma \frac{\partial |\mathbf{u}|^2}{\partial x_j} \right) \frac{D \Delta_j}{D t}, \quad (44)$$

where γ denotes the skewness of the filter. Skewness has been explicitly incorporated, since the commutator error exhibits both diffusive and dispersive behaviors in case skewed filters are applied. In terms of (44) the $-c_1 \gamma \partial_j |\mathbf{u}|^2$ part accounts for this dispersive effect. The other term in (44) represents the contributions associated with strictly symmetric filters.

The Lagrangian modeling (44) has been tested *a priori* using DNS data of a temporal mixing layer. The results indicated the accuracy of the proposed model for the transport of resolved kinetic energy by the commutator error. The commutator-error dispersion is found to be considerable in case $|\gamma| \gtrsim \frac{1}{10}$. These additional effects could be successfully captured by the dispersive part in (44). The optimal ratio between the constants c_1 and c_0 is in the range 10–30. A dynamic evaluation of these parameters may be contemplated in future implementations of this model.

The Lagrangian context also suggests an explicit model for the convective flux commutator $C_j(u_i u_j)$. We performed an *a priori* testing of this new model and compared it to other CE models based on similarity and gradient formulations.⁷ The results showed that the Lagrangian commutator-error model correlates less well in case symmetric filters are applied. For the skewed case the Lagrangian CE-model correlates roughly comparably to the other two models. The similarity and gradient models are well known for their high levels of correlation. This indicates that the

spatial structure of the commutator error is better captured by one of these two models than by the Lagrangian model. However, the similarity and gradient models are known to fail to represent important aspects of the subfilter dynamics. In particular, too many small scales are generated in simulations using the similarity model while the gradient model may be responsible for inducing instabilities in the large-eddy simulation. By construction, the new Lagrangian model does properly capture the underlying dynamics of the commutator error. The accuracy with which the Lagrangian model captures commutator-error dynamics in actual LES is a topic of future investigations.

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- ¹B. J. Geurts, *Elements of Direct and Large-Eddy Simulation* (Edwards, Ann Arbor, 2003).
- ²S. B. Pope, *Turbulent Flows* (Cambridge University Press, Cambridge, UK, 2000).
- ³C. Meneveau and J. Katz, "Scale-invariance and turbulence models for large-eddy simulation," *Annu. Rev. Fluid Mech.* **32**, 1 (2000).
- ⁴A. W. Vreman, B. J. Geurts, and H. Kuerten, "Large-eddy simulation of the turbulent mixing layer," *J. Fluid Mech.* **339**, 357 (1997).
- ⁵S. Ghosal and P. Moin, "The basic equations for the large eddy simulation of turbulent flows in complex geometry," *J. Comput. Phys.* **118**, 24 (1995).
- ⁶B. J. Geurts, A. W. Vreman, J. G. M. Kuerten, and R. van Buuren, "Non-commuting filters and dynamic modeling for LES of turbulent compressible flow in 3d shear layers," in *Direct and Large-Eddy Simulation II*, edited by J. P. Chollet, P. R. Voke, and L. Kleiser (Kluwer Academic, Dordrecht, 1997), pp. 47–56.
- ⁷F. van der Bos and B. J. Geurts, "Commutator-errors in the filtering approach to large-eddy simulation," *Phys. Fluids* **17**, 035108 (2005).
- ⁸B. J. Geurts, "How can we make Large Eddy Simulation to fulfill its promise?" in *Advances in LES of Complex Flows*, edited by R. Friedrich and W. Rodi (Kluwer Academic, Dordrecht, 2002), pp. 13–32.
- ⁹S. Ghosal, "Mathematical and Physical Constraints on Large-Eddy Simulation," *AIAA J.* **37**, 425 (1999).
- ¹⁰B. J. Geurts, A. W. Vreman, and J. G. M. Kuerten, "Comparison of DNS and LES of transitional and turbulent compressible flow: flat plate and mixing layer," in *AGARD Conference Proceedings 551: Application of Direct and Large Eddy Simulation to Transition and Turbulence* (Canada Communication Group, Hull (Quebec), 1994), page 5.
- ¹¹A. J. Riley and M. V. Lowson, "Development of a three dimensional free shear layer," *J. Fluid Mech.* **369**, 49 (1998).
- ¹²O. V. Vasilyev and D. E. Goldstein, "Local spectrum of commutation error in large eddy simulations," *Phys. Fluids* **16**, 470 (2004).
- ¹³O. V. Vasilyev, T. S. Lund, and P. Moin, "A General Class of Commutative Filters for LES in Complex Geometries," *J. Comput. Phys.* **146**, 82 (1998).
- ¹⁴H. van der Ven, "A family of large eddy simulations LES filters with nonuniform filter widths," *Phys. Fluids* **7**, 1171 (1995).
- ¹⁵S. Ghosal, "An analysis of numerical errors in large-eddy simulations of turbulence," *J. Comput. Phys.* **125**, 187 (1996).
- ¹⁶B. J. Geurts and J. Fröhlich, "A framework for predicting accuracy limitations in large-eddy simulation," *Phys. Fluids* **14**, L41 (2002).
- ¹⁷J. Meyers, B. J. Geurts, and M. Baelmans, "Database-analysis of errors in large-eddy simulations," *Phys. Fluids* **15**, 2740 (2003).
- ¹⁸F. K. Chow and P. Moin, "A further study of numerical errors in large-eddy simulations," *J. Comput. Phys.* **184**, 366 (2003).
- ¹⁹J. Gullbrand and F. K. Chow, "The effect of numerical errors and turbulence models in large-eddy simulation of turbulent channel flow, with and without explicit filtering," *J. Fluid Mech.* **495**, 323 (2003).

- ²⁰F. van der Bos, B. Tao, C. Meneveau, and J. Katz, "Effects of small-scale turbulent motions on the filtered velocity gradient tensor as deduced from holographic particle image velocimetry measurements," *Phys. Fluids* **14**, 2456 (2002).
- ²¹J. Bardina, J. H. Ferziger, and W. C. Reynolds, "Improved turbulence models based on LES of homogeneous incompressible turbulent flows,"

Department of Mechanical Engineering, Stanford University, Stanford, Technical Report No. TF-19, 1984.

- ²²R. A. Clark, J. H. Ferziger, and W. C. Reynolds, "Evaluation of subgrid-scale models using an accurately simulated turbulent flow," *J. Fluid Mech.* **91**, 1 (1979).