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Numerically induced high-pass dynamics in large-eddy simulation

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The numerical distortion of the smallest resolved-scale dynamics in large-eddy simulation may be understood in terms of the filter that is induced by the spatial discretization. At marginal subfilter resolution $r=\Delta/h$, with filter width Δ and grid spacing h , the character of the large-eddy closure problem is strongly influenced by the numerical method. We show that additional high-pass contributions arise from the spatial discretization. The relative importance of, on the one hand, the turbulent stresses and, on the other hand, the numerically induced contributions, is quantified for general finite differencing methods. We derive and analyze the induced filters for several popular discretization methods, including higher order central and upwind methods. The application of these induced filters to small-scale turbulent flow structures gives rise to a characteristic amplitude reduction and phase shift. Their dynamic relevance is quantified in terms of the subfilter resolution. The numerical high-pass effects are found to be negligible if the subfilter resolution is large enough ($r \gtrsim 4$). Conversely, the numerically induced effects are comparable to, or even larger than the turbulent stresses as $r=1-2$. © 2005 American Institute of Physics. [DOI: [10.1063/1.2140022](https://doi.org/10.1063/1.2140022)]

I. INTRODUCTION

Direct numerical simulation and large-eddy simulation are two important strategies for the numerical investigation of turbulent flows. Within the constraints of present-day computing infrastructure, most turbulent flows of interest to science and technology contain too many scales for a direct numerical simulation to be feasible.^{1,2} Instead, the direct simulation approach is adopted for full resolution of flow problems of modest complexity; e.g., to underpin theoretical and modeling studies.

The principal computational limitations associated with direct numerical simulation motivate the introduction of large-eddy simulation.^{3,4} The focus in large-eddy simulation is on a computationally more accessible coarsened flow description. The coarsening is obtained by applying a low-pass spatial filter with filter width Δ to the governing equations. In turn, this allows an external control over the required spatial resolution, and only the primary flow features are explicitly resolved. The spatial filtering of the nonlinear terms gives rise to the well-known closure problem for the turbulent stress which encompasses the dynamic effects of the filtered-out small scales on the retained length scales. Viewed entirely from the PDE level corresponding to the spatially filtered Navier-Stokes equations, the remaining task is to close the system of equations by modeling these small-scale dynamic effects in terms of the resolved flow. Considerable effort has been put into construction, testing, and tuning of

such models for the small-scale turbulent flow features over the past years.^{2,3,5}

The above sketch of large-eddy simulation is incomplete in one important respect as it does not contain the unavoidable subsequent discretization step. In fact, since the numerical representation is typically associated with only marginal resolution, a significant alteration of the resolved scales' dynamics may be introduced in the computational model.^{1,6-9} It is the purpose of this paper to quantify the numerical error dynamics explicitly for a number of characteristic, well-known discretization methods. The specification of the numerical method implies, next to the filter width Δ , the introduction of a second length scale h that characterizes the (local) computational grid spacing. Correspondingly, this discretization step induces a second element of possible flow filtering which translates into additional contributions to the closure problem. In this paper we consider these combined filtering effects in detail in terms of the *modified* equation. We identify the full closure of the "computational turbulent stress tensor," which entails both the turbulent stresses as well as contributions due to the numerical method. Specifically, we identify the numerical discretization effects associated with central and upwind differencing methods, complementing literature on so-called "implicit filtering" in large-eddy simulation in Refs. 1 and 10–12.

The numerical distortion in large-eddy simulation alters the appreciation of the small-scale dynamics and may even cross over to the large flow features that carry most of the kinetic energy of the flow.^{13,14} The relative importance of the dynamic consequences due to the numerically induced filter

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and the turbulent stresses depend strongly on the subfilter resolution $r=\Delta/h$. If r is sufficiently large, the grid-independent large-eddy solution consistent with the assumed value of Δ may be accurately approximated. However, large-eddy simulation of applications with a realistic complexity is typically associated with marginal resolution corresponding to $r=1-2$. In that case the numerically induced effects are comparable to or even larger than the turbulent stresses for typical discretization methods such as central or upwind finite difference or finite volume methods. Thereby, the computational large-eddy closure typically contains an important contribution that is sensitive to the adopted spatial discretization.

The problem of the possible interference between numerical discretization errors and errors due to the adopted subgrid modeling of the turbulent stresses has been addressed in a number of ways in recent years, ranging from analytical⁶ to *a posteriori* studies.^{8,9,15,16} A formalism for analyzing errors in turbulent flow problems was developed by Ghosal.⁶ Analytical expressions for the power spectra of the errors were obtained within the so-called joint-normal approximation for turbulent velocity fields.¹⁷ In the work by Ghosal, a nonlinear analysis involving a broad spectrum of length scales was presented. In order to gain some independent control over the discretization errors, it was suggested to implement large-eddy models with a filter width that is greater than the grid spacing. In terms of the subfilter resolution r , this corresponds to $r>1$. In the same year, Vreman *et al.*¹⁵ presented a large-eddy simulation study of turbulent mixing in which the ratio between filter width and grid spacing was varied. This confirmed the strong effects of the adopted spatial discretization method in case $r=1$ and showed that the different errors may counteract, thereby leading to smaller total errors because of a “fortuitous” cancellation. These basic observations suggest using larger values of r . However, this contrasts sharply with the practical complication that such values of r require significantly higher computational effort than may be available for studying actual complex flow applications.

The role numerical discretization errors may have in situations of marginal resolution has triggered a strong interest in implicit filtering approaches (see, e.g., Refs. 18 and 19). In these approaches the flow smoothing that arises from the application of a spatial discretization method was exploited as part of the large-eddy modeling. By adopting dissipative numerical methods in combination with $r=1$, the need for introducing a separate dissipative subgrid model was considered no longer required. An important example of this approach is known as MILES (monotonically integrated large-eddy simulation).¹⁸ More recent developments²⁰ have indicated that the leading truncation error in certain discretization methods can be identified with certain explicit subgrid-scale models. This allows to implement and interpret the main contributions of this class of subgrid-scale models as part of the numerical modeling and is referred to as implicit modeling.

In this paper we complement these studies by explicitly determining the filters that are induced by a number of popular discretization methods. Moreover, we quantify and com-

pare the exact turbulent stresses and the numerically induced filtering contributions. This confirms that the induced filtering effect and the turbulent stresses are *both* of importance in cases where practically feasible values $r=1-2$ are considered. The total closure problem in the computational model is shown to account for (i) the coarseness of the numerical representation, (ii) the type of the discretization, and (iii) the traditional turbulent stress tensor. The first two contributions may be expressed in terms of an explicit high-pass filter associated with the numerical treatment. The third contribution is commonly approached by introducing an explicit subgrid model. The comparison of the magnitude of the different contributions appears to advocate separate modeling of the turbulent stress tensor, *next to* explicit incorporation of the numerical high-pass filter contributions. This route offers an independent control over the various sources of error in large-eddy simulation which distinguishes it from the strict implicit modeling approach, where the numerical truncation error is meant to correspond to a particular subgrid model, and, vice versa, where some appropriately selected subgrid model would prescribe the use of a particular numerical method. Moreover, the principal possibility to achieve a grid-independent large-eddy solution⁸ corresponding to a fixed value of the filter width Δ is retained, while it is lost in the implicit modeling formulation as the effective dissipation arising from the numerical method is reduced whenever the grid is refined. In such cases, the limiting situation that arises as the grid spacing tends to zero is that of direct numerical simulation.

The organization of this paper is as follows. In Sec. II we describe the filtering approach to large-eddy simulation and focus in particular on the additional contributions to the turbulent stresses due to the filter that is induced by the spatial discretization. Section III is devoted to the derivation of the induced filter associated with general central finite differencing and (higher order) upwind methods. The magnitude of the contributions to the numerical turbulent stress tensor due to the spatial discretization is analyzed and discussed in Sec. IV. Finally, in Sec. V some concluding remarks are collected.

II. DECOMPOSITION OF THE NUMERICAL TURBULENT STRESS TENSOR

In this section we first briefly recall the spatial filtering approach to large-eddy simulation. We then identify the filter that is induced by a spatial discretization method. This allows to discuss the closure problem in the computational model in terms of the equivalent *modified* partial differential equation.¹ The total closure problem is formulated in terms of the computational turbulent stress tensor, which is shown to contain a characteristic high-pass filter contribution next to the well-known turbulent stress tensor.

Filtering the Navier-Stokes equations requires a low-pass spatial filter L . Often, a convolution filter is adopted, which in one spatial dimension associates the filtered velocity $\bar{u}$ with the unfiltered velocity u through

$$\bar{u}(x) = L(u, x; \lambda) = \int_{-\infty}^{\infty} g(\xi - x, \lambda) u(\xi) d\xi \quad (1)$$

with normalized filter kernel $g(z, \lambda)$; i.e., $L(c) = c$ for any constant function c . In three dimensions one commonly adopts product filters that arise from the composition of three separate one-dimensional filters corresponding to each of the coordinate directions.³ A filter kernel is characterized by an externally specified length scale parameter λ , which defines the effective filter width Δ ; e.g., as²²

$$\frac{1}{\Delta} = \int_{-\infty}^{\infty} g^2(z, \lambda) dz. \quad (2)$$

This definition applies to all kernels that are square integrable.³ Other definitions proposed in literature (see Ref. 2 for an overview) are more restricted in their applicability to different filters. As an example, the top-hat filter ℓ is given by

$$\bar{u} = \ell(u, x; a, b) = \int_{x+a}^{x+b} \frac{u(\xi)}{b-a} d\xi, \quad (3)$$

for which $\Delta = b - a$. The top-hat filter in (3) is called symmetric if $a = -b < 0$, but this definition also allows for general asymmetric or “skewed” filters^{23,24} for which x is not the central point of the integration interval. We will show in Sec. III that the induced filter of a general finite differencing method may be expressed as a linear combination of local top-hat filters.

For incompressible fluids, the application of a filter L to the continuity and Navier-Stokes equations leads to

$$\begin{aligned} \partial_j \bar{u}_j &= 0, \\ \partial_t \bar{u}_i + \partial_j (\bar{u}_j \bar{u}_i) + \partial_i \bar{p} - \frac{1}{\text{Re}} \partial_{jj} \bar{u}_i &= -\partial_j (\overline{u_i u_j} - \bar{u}_i \bar{u}_j). \end{aligned} \quad (4)$$

Here ∂_i (∂_j) denotes partial differentiation with respect to time t (spatial coordinate x_j), and summation over repeated indices is implied. The component of the filtered velocity in the x_j direction is $\bar{u}_j$ and $\bar{p}$ is the filtered pressure. Finally, “Re” denotes the Reynolds number. In this formulation we recognize the application of the Navier-Stokes operator to the filtered solution $\{\bar{u}_j, \bar{p}\}$ on the left-hand side. On the right-hand side, the central closure problem is expressed by the divergence of the turbulent stress tensor

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j. \quad (5)$$

This tensor cannot be calculated from the filtered solution alone. Hence, one of the aims in the development of large-eddy simulation is the effective capturing of the primary dynamical effects of τ_{ij} in terms of model tensors that can be expressed in terms of the filtered solution alone. The turbulent stress tensor concisely represents the closure problem on the PDE level of filtered Navier-Stokes equations.

With the application of the spatial large-eddy filter, scales smaller than the filter width Δ are effectively removed from the description. This motivates the use of a grid spacing h on the order Δ instead of resolving the Kolmogorov dissi-

pation length scale $\eta \ll \Delta$, as would be required for direct simulation. However, in general it is unclear what subfilter resolutions $r = \Delta/h$ are acceptable from the point of view of numerical reliability of the simulations. In practice, one frequently observes that the subfilter resolution r is taken as low as 1 or 2.^{8,15,25,26} In such cases the smallest retained flow features are only marginally resolved and one may anticipate a significant effect from the numerical discretization.^{9,16} Hence, even though the numerical filtering component can be controlled in principle by choosing r sufficiently large, virtually all large-eddy studies reported in literature contain dynamic contributions arising from the coarseness of the discretization.^{1,10,11}

The additional small-scale effects arising from the induced numerical filter should be fully included into the analysis of the large-eddy equations. This advocates considering the closure problem at the level of the actual computational model; i.e., after the spatial discretization has been incorporated. Such an approach differs markedly from addressing the closure problem in terms of the turbulent stresses as arise on the PDE level of filtered Navier-Stokes equations. The most important aspects of this “computational turbulent stress” closure problem can be readily appreciated in terms of the one-dimensional inviscid Burgers equation to which we turn next.

The most important characteristics of a computational large-eddy model may be expressed by introducing the discrete convective flux $\delta_x(\bar{u}^2)$ associated with the spatial discretization operator δ_x . Relative to this discrete flux, we may group the remainder into the extended closure problem. To further clarify the associated closure problem we recall that the discrete derivative operator, e.g., corresponding to finite differencing, can be expressed as $\delta_x f = \partial_x \hat{f}$, where $\hat{f}$ denotes the filtering of f with the numerically induced filter $(\hat{\cdot})$.¹ Within this representation, we may write the filtered inviscid Burgers equation in one spatial dimension as

$$\begin{aligned} \partial_t \bar{u} + \frac{1}{2} \partial_x (\bar{u}^2) &= \partial_t \bar{u} + \frac{1}{2} \delta_x (\bar{u}^2) + \frac{1}{2} [\partial_x (\bar{u}^2) - \delta_x (\bar{u}^2)] \\ &= \partial_t \bar{u} + \frac{1}{2} \delta_x (\bar{u}^2) + \frac{1}{2} \partial_x (\bar{u}^2 - \hat{u}^2) \\ &= \partial_t \bar{u} + \frac{1}{2} \partial_x (\hat{u}^2) + \frac{1}{2} \partial_x (\xi) = 0, \end{aligned} \quad (6)$$

in which we introduced the *computational turbulent stress tensor* $\xi = \bar{u}^2 - \hat{u}^2$, which constitutes the full closure problem including the contributions due to the spatial discretization. We observe that the combined action of spatial discretization and large-eddy filtering gives rise to an equivalent *modified equation*³ in which an additional term emerges that involves the induced numerical filter $(\hat{\cdot})$ applied to $\bar{u}^2$. Hence, instead of a tensor τ , the computational stress tensor ξ appears in the modified equation. In order to understand the dynamics of the full computational model, this modified equation provides an important point of departure, as already emphasized by Rogallo and Moin.¹ In (6) the solution $\bar{u}$ is defined as a continuous function of x . In actual numerical formulations, the solution is typically represented as a discrete-grid function. This may lead to another source of numerical error associated with aliasing. If the solution $\bar{u}$ is represented on a

grid then only a finite number of length scales can be supported. The product $\bar{u}^2$ may, however, contain additional length scales that fall outside this “grid-supported range.” These contribute to the aliasing error, which is explicitly discussed in Ref. 6. In this paper we will analyze the different contributions for individual modes only, and aliasing errors will not be investigated.

There are several ways to split the numerical turbulent stress tensor ξ into its characteristic contributions.^{27,28} The relation with the closure problem for τ on the PDE level is expressed most directly by

$$\xi = \bar{u}^2 - \hat{u}^2 = (\bar{u}^2 - \bar{u}^2) + (\bar{u}^2 - \hat{u}^2) = \tau + \mathcal{H}(\bar{u}^2), \quad (7)$$

where $\mathcal{H}(f) = f - \hat{f}$ denotes the high-pass filter associated with $(\hat{\cdot})$. Since the high-pass filter operates on $\bar{u}^2$, which is available during the simulation, this term does not constitute a separate closure problem. Consistent with this decomposition, subgrid modeling of ξ in the modified equation would hence involve modeling of τ by a subgrid model $m(\bar{u})$ and evaluation of the numerical high-pass filter acting on $\bar{u}^2$. We remark that next to the discretization of the convective terms, the numerical treatment of the viscous flux and the flux due to an assumed subgrid model $m(\bar{u})$ may also contribute important sources of error. For these particular contributions to the numerical error, the filter induced by the spatial discretization method needs to be taken into consideration as well. This may be done following the same steps as will be illustrated for the convective terms.

The difference between ξ for a given discretization method, and τ depends on the subgrid resolution that characterizes the strength of the numerical filtering. If the subgrid resolution r is sufficiently large, the numerical filter operator $(\hat{\cdot})$ approaches the identity operator for all length scales relevant to τ . Hence, as follows from (7), this implies that $\xi \rightarrow \tau$, and consequently (6) reduces to the filtered inviscid Burgers equation. In practical situations the grid spacing is chosen such that r assumes quite modest values and the numerical filter component in the full closure problem needs to be explicitly accounted for. The influence of the spatial discretization is often referred to as implicit filtering in literature (e.g., Refs. 10 and 11).

In three spatial dimensions the decomposition of the computational stress tensor may be expressed quite analogously. We consider spatial discretization methods that are given by weighted finite differencing schemes on uniform Cartesian grids³ to illustrate the required steps. This class of schemes includes several well-known finite volume methods and is used in various direct and large-eddy simulation studies. In these methods one does not apply the finite differencing operator directly to the solution u but instead first performs an additional surface-averaging over the two directions that are perpendicular to the direction in which one wants to calculate a partial derivative. The induced numerical filter corresponding to, e.g., the discretization in the x_1 direction may be denoted by $\delta_1 f = \partial_1(\hat{f}^{(1)})$, where $(\hat{\cdot})^{(1)}$ represents the filtering effects associated with finite differencing in the x_1 direction as well as due to spatial averaging over the x_2 and x_3 directions. Correspondingly, the induced nu-

merical filter may differ for each of the coordinate directions; this complication was considered earlier by Lund.¹¹ Following the steps outlined in (6), we may hence write the filtered convective fluxes as

$$\partial_j(\bar{u}_i \bar{u}_j) = \delta_j(\bar{u}_i \bar{u}_j) + \partial_j(\bar{u}_i \bar{u}_j - \widehat{\bar{u}_i \bar{u}_j}^{(j)}) = \partial_j(\widehat{\bar{u}_i \bar{u}_j}^{(j)}) + \partial_j \xi_{ij}. \quad (8)$$

This decomposition of the filtered convective fluxes allows us to write the computational turbulent stress tensor ξ_{ij} analogous to (7) as (no sum over j here)

$$\begin{aligned} \xi_{ij} &= \bar{u}_i \bar{u}_j - \widehat{\bar{u}_i \bar{u}_j}^{(j)} = (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) + (\bar{u}_i \bar{u}_j - \widehat{\bar{u}_i \bar{u}_j}^{(j)}) \\ &= \tau_{ij} + \mathcal{H}_j(\bar{u}_i \bar{u}_j), \end{aligned} \quad (9)$$

in which the turbulent stress tensor τ_{ij} , as well as the numerically induced contributions arise in terms of the high-pass filter $\mathcal{H}_j(f) = f - \hat{f}^{(j)}$ associated with the numerical treatment in the x_j direction. If we assume in (9) that the discretization and computational grid are the same in each direction, then one may restrict to a single high-pass operator $\mathcal{H}$. We will specify weighted finite differencing methods and the total induced filters $(\hat{\cdot})^{(j)}$ in more detail in the next section. A further extension to finite volume methods on general curvilinear meshes can be developed as well. This requires a more involved system of notation which mainly contributes to technical complications in the exposition. We will not include this here as all main aspects of the extension to more dimensions are already addressed for weighted finite differencing schemes. We turn our attention to the induced numerical filter in the next section and address the dynamic implications in Sec. IV.

III. SPATIAL DISCRETIZATION AND INDUCED FILTER

In this section we will first derive the induced filter associated with general (weighted) finite differencing methods. The Fourier transform of the induced filter kernel is then analyzed for higher-order central and upwind discretization methods. We show that the induced filter may be expressed as a linear combination of top-hat filters and present the corresponding spectral dependency of the filter characteristics. Central schemes result in a reduction of the amplitude while an additional phase error is introduced in case skewed upwind methods are considered.

The induced filter associated with a spatial discretization method was defined earlier according to $\delta_x f = \partial_x \hat{f}$. We determine this filter for a general class of spatial discretization methods and consider a uniform grid with mesh spacing h for convenience. Specifically, we focus on the finite differencing methods $\delta_x^{(-n,m)}$:

$$\delta_x^{(-n,m)} f(x) = \sum_{j=-n}^m \frac{a_j}{h} f(x + jh). \quad (10)$$

These methods use a stencil that covers the interval $[x - nh, x + mh]$ and includes $m+n+1$ grid points. We consider $m \geq 0$ and $n \geq 0$ with $m+n \geq 1$. The discretization weights $\{a_j\}$ are such that a consistent scheme is obtained; i.e.,

$$\sum_{j=-n}^m a_j = 0. \quad (11)$$

The induced numerical filter can be expressed in terms of a weighted sum of local top-hat filters, as will be shown next. In fact, we may write

$$\begin{aligned} h\delta_x^{(-n,m)}f(x) &= a_m\{f(x+mh) - f[x+(m-1)h]\} + (a_m + a_{m-1}) \\ &\quad \times \{f[x+(m-1)h] - f[x+(m-2)h]\} \\ &\quad + (a_m + a_{m-1} + a_{m-2})\{f[x+(m-2)h] \\ &\quad - f[x+(m-3)h]\} + \cdots \\ &\quad + (a_m + a_{m-1} + \cdots + a_{-n+1}) \\ &\quad \times \{f[x-(n-1)h] - f(x-nh)\}, \end{aligned} \quad (12)$$

which may be regrouped concisely as

$$\delta_x^{(-n,m)}f(x) = \frac{1}{h} \sum_{j=-n+1}^m b_j \{f(x+jh) - f[x+(j-1)h]\}, \quad (13)$$

where

$$b_j = \sum_{i=j}^m a_i; \quad j = -n+1, \dots, m. \quad (14)$$

The contribution of each interval $[x+(j-1)h, x+jh]$ may be represented as

$$\begin{aligned} \frac{1}{h} \{f(x+jh) - f[x+(j-1)h]\} \\ = \partial_x \left(\int_{x+(j-1)h}^{x+jh} \frac{1}{h} f(s) ds \right) = \partial_x \{\ell[f, x; (j-1)h, jh]\}, \end{aligned} \quad (15)$$

where $\ell[f, x; (j-1)h, jh]$ is the local top-hat filter as defined in (3). The total induced numerical filter can hence be expressed as a weighted average of skewed top-hat filters. In particular,

$$\begin{aligned} \delta_x^{(-n,m)}f(x) &= \sum_{j=-n+1}^m b_j \partial_x \{\ell[f, x; (j-1)h, jh]\} \\ &= \partial_x [\mathcal{L}_{-n,m}(f)], \end{aligned} \quad (16)$$

where $\mathcal{L}_{-n,m}(f) = \hat{f}$ denotes the total induced numerical filter corresponding to the discretization method $\delta_x^{(-n,m)}f$ defined on the stencil $[x-nh, x+mh]$. The properties of specific induced filters will be determined next. First, we consider central finite differencing schemes and turn to upwind schemes momentarily.

The numerical filter as summarized in (16) can be specified more transparently for central finite differencing schemes for which $m=n$, $a_0=0$, and $a_j=-a_{-j}$, $j=1, \dots, n$. Correspondingly, (10) can be rewritten as

$$\begin{aligned} \delta_x^{(-n,n)}f(x) &= \sum_{j=-n}^n \frac{a_j}{h} f(x+jh) \\ &= \sum_{j=1}^n d_j \left(\frac{f(x+jh) - f(x-jh)}{2jh} \right), \end{aligned} \quad (17)$$

where we set $d_j=2ja_j$. In terms of symmetric top-hat filters, we may express this as

$$\delta_x^{(-n,n)}f(x) = \sum_{j=1}^n d_j \partial_x [\ell(f, x; -jh, jh)] = \partial_x [\mathcal{L}_{-n,n}(f)]. \quad (18)$$

As an example, for the second-order central discretization we have

$$\delta_x^{(-1,1)}f(x) = \frac{1}{2h} [f(x+h) - f(x-h)], \quad (19)$$

which corresponds to $n=1$ and $a_1=-a_{-1}=1/2$, such that $d_1=2a_1=1$. Hence, we find

$$\begin{aligned} \delta_x^{(-1,1)}f(x) &= \partial_x \left(\int_{x-h}^{x+h} \frac{f(s)}{2h} ds \right) = \partial_x [\ell(f, x; -h, h)] \\ &= \partial_x [\mathcal{L}_{-1,1}(f)]. \end{aligned} \quad (20)$$

The induced filter $\mathcal{L}_{-1,1}(f) = \ell(f, x; -h, h)$; i.e., a top-hat filter with filter width equal to twice the grid spacing h . The fourth-order accurate central differencing method corresponds to $n=2$, and may be written as

$$\begin{aligned} \delta_x^{(-2,2)}f(x) &= \frac{1}{12h} [-f(x+2h) + 8f(x+h) - 8f(x-h) \\ &\quad + f(x-2h)] \\ &= \frac{4}{3} \left(\frac{f(x+h) - f(x-h)}{2h} \right) \\ &\quad - \frac{1}{3} \left(\frac{f(x+2h) - f(x-2h)}{4h} \right), \end{aligned} \quad (21)$$

from which we infer that $d_1=4/3$ and $d_2=-1/3$. Hence, the induced filter $\mathcal{L}_{-2,2}$ corresponding to $\delta_x^{(-2,2)}f(x)$ may be written as

$$\begin{aligned} \delta_x^{(-2,2)}f(x) &= \partial_x \left[\frac{4}{3} \ell(f, x; -h, h) - \frac{1}{3} \ell(f, x; -2h, 2h) \right] \\ &= \partial_x [\mathcal{L}_{-2,2}(f)]. \end{aligned} \quad (22)$$

A less well-known example in this sequence is the sixth-order discretization scheme. This corresponds to $n=3$ and may be written as

FIG. 1. The filter kernel $g_{-n,n}$ multiplied by the grid spacing h is shown in (a), and the Fourier transform $G_{-n,n}$ of the induced numerical filter corresponding to second-order accurate central differencing is shown in (b) at $n=1$ (solid), $n=2$ (dashed), and $n=3$ (dash-dotted).

$$\begin{aligned}
 \delta_x^{(-3,3)} f(x) &= \frac{1}{60h} [f(x+3h) - 9f(x+2h) + 45f(x+h) \\
 &\quad - 45f(x-h) + 9f(x-2h) - f(x-3h)] \\
 &= \frac{3}{2} \left(\frac{f(x+h) - f(x-h)}{2h} \right) \\
 &\quad - \frac{3}{5} \left(\frac{f(x+2h) - f(x-2h)}{4h} \right) \\
 &\quad + \frac{1}{10} \left(\frac{f(x+3h) - f(x-3h)}{6h} \right) \\
 &= \partial_x \left(\frac{3}{2} \ell(f, x; -h, h) - \frac{3}{5} \ell(f, x; -2h, 2h) \right. \\
 &\quad \left. + \frac{1}{10} \ell(f, x; -3h, 3h) \right), \quad (23)
 \end{aligned}$$

from which we infer that $d_1=3/2$, $d_2=-3/5$, and $d_3=1/10$.

To characterize the induced filters, we may determine the effective filter width $\Delta_{-n,n}$ of $\mathcal{L}_{-n,n}(f)$ as defined by (2). Following (1), the kernels $g_{-n,n}$ of the induced filters $\mathcal{L}_{-n,n}$ are piecewise constant functions on the interval $[-nh, nh]$ and 0 outside. These kernels may readily be inferred from the corresponding combination of top-hat filters that is involved. After some calculation, we find

$$g_{-1,1}(z) = \frac{1}{2h}; \quad |z| < h, \quad (24)$$

$$g_{-2,2}(z) = \begin{cases} \frac{7}{12h}, & |z| < h, \\ -\frac{1}{12h}, & h < |z| < 2h, \end{cases} \quad (25)$$

$$g_{-3,3}(z) = \begin{cases} \frac{37}{60h}, & |z| < h, \\ -\frac{2}{15h}, & h < |z| < 2h, \\ \frac{1}{60h}, & 2h < |z| < 3h. \end{cases} \quad (26)$$

These kernels are illustrated in Fig. 1(a). Both positive and negative values may occur if $n \geq 2$. The corresponding effective filter widths are found to be $\Delta_{-1,1}/h=2$, $\Delta_{-2,2}/h=36/25=1.44$, and $\Delta_{-3,3}/h=300/239 \approx 1.2552\dots$. We observe that an increase in the order of the finite differencing scheme implies a decrease in the effective filter width of the induced filter. For comparably large flow structures relative to the filter width $\Delta_{-n,n}$, this trend implies that the induced filtering effect will be uniformly diminished. In particular, with an increase in the order the induced filtering is less effective, and for a larger range of flow structures. The effect on small-scale structures can not be fully characterized by $\Delta_{-n,n}$ alone. Instead, the behavior of the Fourier transform of the induced filter kernels is required, to which we turn next.

The induced filter corresponding to $\delta_x^{(-n,n)}$ may be concisely characterized by investigating the effect on a Fourier mode. To specify the induced filtering of e^{iKx} , we first notice that

$$\ell(e^{iKx}, x; -nh, nh) = \left(\frac{\sin(nKh)}{nKh} \right) e^{iKx} = \Gamma(nKh) e^{iKx}, \quad (27)$$

where $\Gamma(z) = \sin(z)/z$ is the Fourier transform of the kernel of the symmetric top-hat filter. This basic rule allows us to write $\mathcal{L}_{-n,n}(e^{iKx}) = G_{-n,n}(Kh) e^{iKx}$, in which

$$G_{-1,1}(Kh) = \Gamma(Kh), \quad (28)$$

$$\mathcal{G}_{-2,2}(Kh) = \frac{4}{3}\Gamma(Kh) - \frac{1}{3}\Gamma(2Kh), \quad (29)$$

$$\mathcal{G}_{-3,3}(Kh) = \frac{3}{2}\Gamma(Kh) - \frac{3}{5}\Gamma(2Kh) + \frac{1}{10}\Gamma(3Kh). \quad (30)$$

In Fig. 1(b) we plotted the Fourier transform $\mathcal{G}_{-n,n}$ of the induced kernels of $\mathcal{L}_{-n,n}$ as a function of Kh . We notice that the filter corresponding to a higher-order spatial discretization is itself a higher-order filter; with increasing order, the Fourier transform of the kernel is seen to stay closer to the identity operator for a wider range of wave numbers.^{21,22,24} Each discretization method gives rise to a particular damping of the amplitude of individual modes, which induces a specific dynamic contribution in an actual large-eddy simulation based on this method. The role of the total filter is discussed further in, e.g., Refs. 21 and 24.

The induced filter associated with weighted finite differencing in three spatial dimensions can be specified largely analogously to the treatment in one dimension given above. We will next present the approximation of the partial derivative in the x direction in a three-dimensional context; corresponding expressions associated with the other two directions are similar.

The approximation of $\partial_x f$ in the grid point (x_i, y_j, z_k) is denoted by $(D_x f)_{ijk}$. Weighted finite differencing methods are defined through

$$(D_x f)_{ijk} = \{\delta_x^{(-n,m)}[L_{yz}(f)]\}_{ijk} = (\partial_x \{\mathcal{L}_{-n,m}[L_{yz}(f)]\})_{ijk}, \quad (31)$$

where we introduced the “surface-averaging” L_{yz} to denote additional filtering over y and z . Hence, weighted finite differencing schemes are built around the well-known finite differencing operator $\delta_x^{(-n,m)}$, which, however, now acts on a surface-averaged field $L_{yz}(f)$ instead of on f directly. This additional averaging allows one to arrive at a more robust high-order implementation of the numerical derivatives, compared to simple finite differencing.^{15,29} One may readily infer from (31) that the total induced numerical filter $(\hat{\cdot})^{(1)}$, as introduced in the previous section, consists of the induced filter $\mathcal{L}_{-n,m}$ arising from $\delta_x^{(-n,m)}$ as well as extra filtering associated with the surface averaging over the y and z directions. This combination of filters needs to be accounted for in three-dimensional applications, as it expresses the differences between the tensors ξ_{ij} and τ_{ij} in (9).

The surface-averaging L_{yz} is usually defined as a “grid filter.” In the point (x_i, y_j, z_k) , it may be expressed as

$$[L_{yz}(f)]_{ijk} = \int dY dZ G_{jk}(Y, Z) f(x_i, Y, Z), \quad (32)$$

where the kernel $G_{jk}(Y, Z)$ is defined in terms of the stencil $[y_{j-n_y}, y_{j+m_y}] \times [z_{k-n_z}, z_{k+m_z}]$ with specific integer pairs (n_y, m_y) and (n_z, m_z) for the y and z directions, respectively. The kernel is given by a collection of Dirac delta functions:

$$G_{jk}(Y, Z) = \sum_{\alpha=-n_y}^{m_y} \sum_{\beta=-n_z}^{m_z} W_{\alpha\beta}^{(jk)} \delta(Y - y_{j+\alpha}) \delta(Z - z_{k+\beta}). \quad (33)$$

The averaging weights $W_{\alpha\beta}^{(jk)}$ correspond to a normalized grid filter; i.e.,

$$\sum_{\alpha=-n_y}^{m_y} \sum_{\beta=-n_z}^{m_z} W_{\alpha\beta}^{(jk)} = 1 \quad (34)$$

for all (j, k) in the grid. If the grid is uniform then the averaging weights are independent of j and k . Moreover, on Cartesian grids it is quite common to restrict to product filters, in which case $W_{\alpha\beta} = w_\alpha w_\beta$ in terms of averaging weights w_α , which define one-dimensional grid filters.

The one-dimensional finite differencing and surface averaging can be combined into some well-known weighted finite differencing schemes. On uniform Cartesian grids, a second-order method arises by combining $\delta_x^{(-1,1)}$ with trapezoidal integration:³⁰

$$(D_x^{(2)} f)_{i,j,k} = (A_{i+1,j,k} - A_{i-1,j,k})/(2h) \quad (35)$$

with

$$A_{i,j,k} = (B_{i,j-1,k} + 2B_{i,j,k} + B_{i,j+1,k})/4$$

and

$$B_{i,j,k} = (f_{i,j,k-1} + 2f_{i,j,k} + f_{i,j,k+1})/4,$$

where h denotes the grid spacing. A fourth-order accurate scheme arises from the combination of $\delta_x^{(-2,2)}$ with a correspondingly more accurate integration rule:¹⁵

$$(D_x^{(4)} f)_{i,j,k} = (-A_{i+2,j,k} + 8A_{i+1,j,k} - 8A_{i-1,j,k} + A_{i-2,j,k})/(12h) \quad (36)$$

with

$$A_{i,j,k} = (-B_{i,j-2,k} + 4B_{i,j-1,k} + 10B_{i,j,k} + 4B_{i,j+1,k} - B_{i,j+2,k})/16$$

and

$$B_{i,j,k} = (-f_{i,j,k-2} + 4f_{i,j,k-1} + 10f_{i,j,k} + 4f_{i,j,k+1} - f_{i,j,k+2})/16.$$

Extensions to nonuniform Cartesian grids can be specified analogously.³¹

The numerical schemes (35) and (36) involve the application of a one-dimensional grid filter Λ for the definition of the filtered fields A_{ijk} and B_{ijk} . The action of these grid filters on a Fourier mode e^{iKx} may be written as

$$\Lambda(e^{iKx}) = e^{iKx} \left(\sum_{\alpha=-n}^m w_\alpha e^{-iK\alpha h} \right); \quad \Lambda(f) = \sum_{\alpha=-n}^m w_\alpha f_\alpha. \quad (37)$$

For the second-order accurate trapezoidal rule, we have $n=m=1$ and $w_{-1}=w_1=1/4$, $w_0=1/2$. Likewise, the fourth-order accurate integration method arises if $n=m=2$ and $w_{-2}=w_2=-1/16$, $w_{-1}=w_1=4/16$, and $w_0=10/16$. The Fourier transforms $\mathcal{G}_n$ of the kernels corresponding to the n th-order integration method may be obtained from (37), and after some calculation we obtain

$$\mathcal{G}_2(Kh) = \frac{1}{2}[1 + \cos(Kh)], \quad (38)$$

$$\mathcal{G}_4(Kh) = \frac{1}{8}[5 + 4\cos(Kh) - \cos(2Kh)].$$

In Fig. 2 these Fourier-transformed kernels are shown. The characteristic reduction of the amplitude of an individual Fourier mode as function of Kh needs to be combined with the corresponding wave-number dependence of the action of

FIG. 2. The Fourier transform of the grid filter $\mathcal{G}_n$ associated with the second-order ($n=2$: solid) and fourth-order ($n=4$: dashed) accurate weighted finite differencing method.

the induced filters $\mathcal{L}_{-n,m}$ in order to identify the total numerical turbulent stress tensor in three spatial dimensions.

So far, only central discretizations were considered. However, in various numerical studies, use is made of discretizations on a skewed stencil.¹⁸ In case an upwind discretization method is adopted, the induced filter is skewed and contributes to both dispersive and dissipative aspects of the smaller resolved scales.^{23,24} To quantify the induced filter of upwind methods in more detail, we first require the effect of a skewed top-hat filter on a Fourier mode e^{iKx} . This is readily obtained as

$$\ell(e^{iKx}, x: -nh, mh) = [\gamma_{-n,m}(Kh) - i\kappa_{-n,m}(Kh)]e^{iKx}, \quad (39)$$

where $\gamma_{-n,m}(z)$ and $\kappa_{-n,m}(z)$ correspond to the real and imaginary parts of the Fourier transform of the kernel of a general top-hat filter, given by

$$\gamma_{-n,m}(z) = \frac{\sin(mz) + \sin(nz)}{(m+n)z}, \quad (40)$$

$$\kappa_{-n,m}(z) = \frac{\cos(mz) - \cos(nz)}{(m+n)z}.$$

If $m=n$, we notice $\gamma_{-n,n}(z) = \Gamma(nz)$ and $\kappa_{-n,n}(z) = 0$, and we reobtain the expression for the symmetric top-hat filter (27). The application of this skewed top-hat filter ℓ to the Fourier mode e^{iKx} can alternatively be expressed as $\ell(e^{iKx}, x: -nh, mh) = A_{-n,m}e^{iK(x-\phi_{-n,m})}$, where the amplitude-reduction $A_{-n,m}$ and phase shift $\phi_{-n,m}$ are given by

$$A_{-n,m}^2(Kh) = \gamma_{-n,m}^2 + \kappa_{-n,m}^2 = \Gamma^2\left(\frac{Kh(m+n)}{2}\right); \quad (41)$$

$$\tan(K\phi_{-n,m}) = \frac{\kappa_{-n,m}}{\gamma_{-n,m}}.$$

Consequently $|A_{-n,m}| \leq 1$ for all Kh and m, n , and $A_{-n,m}(0) = 1$. Moreover, the skewness of the filter induces a phase shift that is zero when the imaginary part $\kappa_{-n,m} = 0$; i.e., in case the filter is symmetric or when $Kh = 0$.

The induced filters corresponding to general upwind discretizations may be obtained in the same way as illustrated above for central discretization. As an example, the first-order forward differencing is given by

$$\begin{aligned} \delta_x^{(0,1)}f(x) &= \frac{1}{h}[f(x+h) - f(x)] = \partial_x[\ell(f, x; 0, h)] \\ &= \partial_x[\mathcal{L}_{0,1}(f)]. \end{aligned} \quad (42)$$

Likewise, the second-order three-point forward differencing may be characterized by

$$\begin{aligned} \delta_x^{(0,2)}f(x) &= \frac{1}{2h}[-f(x+2h) + 4f(x+h) - 3f(x)] \\ &= \frac{3}{2}\left(\frac{f(x+h) - f(x)}{h}\right) \\ &\quad - \frac{1}{2}\left(\frac{f(x+2h) - f(x+h)}{h}\right), \end{aligned} \quad (43)$$

from which the induced filter is readily inferred:

$$\mathcal{L}_{0,2}(f) = \frac{3}{2}\ell(f, x; 0, h) - \frac{1}{2}\ell(f, x; h, 2h). \quad (44)$$

Higher-order examples of forward and backward differencing methods may readily be specified within this framework. The corresponding induced filter kernels $g_{0,n}$ are shown in Fig. 3(a).

The spectral characteristic of the induced filter of a general finite differencing method follows from its application to e^{iKx} . We have for the scheme in (16)

$$\begin{aligned} \mathcal{L}_{-n,m}(e^{iKx}) &= \sum_{j=-n+1}^m b_j \ell[e^{iKx}, x: (j-1)h, jh] \\ &= \sum_{j=-n+1}^m b_j [\gamma_{j-1,j}(Kh) - i\kappa_{j-1,j}(Kh)]e^{iKx} \\ &= [\mathcal{G}_{-n,m}(Kh) - i\mathcal{I}_{-n,m}(Kh)]e^{iKx} \end{aligned} \quad (45)$$

with characteristic functions $\mathcal{G}_{-n,m}$ and $\mathcal{I}_{-n,m}$ given by

$$\begin{aligned} \mathcal{G}_{-n,m}(Kh) &= \sum_{j=-n+1}^m b_j \gamma_{j-1,j}(Kh), \\ \mathcal{I}_{-n,m}(Kh) &= \sum_{j=-n+1}^m b_j \kappa_{j-1,j}(Kh). \end{aligned} \quad (46)$$

This generalizes $\mathcal{L}_{-n,n}$ as specified earlier. For first- and second-order forward differencing $\delta_x^{(0,1)}$ and $\delta_x^{(0,2)}$, the char-

FIG. 3. The induced filter kernel $g_{0,n}$ multiplied by the grid spacing h is shown in (a) corresponding to first-order ($n=1$: solid) and second-order ($n=2$: dashed) forward differencing methods. The characteristic functions $\mathcal{G}_{0,n}$ and $\mathcal{I}_{0,n}$ are shown in (b): $\mathcal{G}_{0,1}$ (solid), $\mathcal{I}_{0,1}$ (dashed), $\mathcal{G}_{0,2}$ (dash-dotted), and $\mathcal{I}_{0,2}$ (dotted).

acteristic functions $\mathcal{G}_{0,n}$ and $\mathcal{I}_{0,n}$ are found explicitly as

$$\mathcal{G}_{0,1}(Kh) = \frac{\sin(Kh)}{Kh}; \quad \mathcal{I}_{0,1}(Kh) = \frac{\cos(Kh) - 1}{Kh}, \quad (47)$$

$$\mathcal{G}_{0,2}(Kh) = \frac{4 \sin(Kh) - \sin(2Kh)}{2Kh}, \quad (48)$$

$$\mathcal{I}_{0,2}(Kh) = \frac{4 \cos(Kh) - \cos(2Kh) - 3}{2Kh},$$

where use was made of (39). In Fig. 3(b) these characteristic functions are plotted. We observe that $|\mathcal{G}_{0,1}| < 1$ for all Kh , while $\mathcal{G}_{0,2}$ is seen to develop an overshoot for a range of modes. If Kh is sufficiently large, $|\mathcal{G}_{0,2}| < 1$ and gradually reduces to 0. The value of $\mathcal{I}_{0,n}$ is seen to be negative and its contribution is quite important for both forward differencing methods. This implies a significant phase shift for a range of wave numbers. The amplitude factor of the full induced filter $\mathcal{A}_{0,n}^2 = \mathcal{G}_{0,n}^2 + \mathcal{I}_{0,n}^2$ is between 0 and 1 for the first-order method, while it assumes values larger than 1 for a range of $|Kh| \leq 3.7175\dots$ for the second-order method, and only reduces to zero if Kh is large enough. Upwind schemes for three-dimensional applications can be constructed along the same lines as adopted for the extension of central schemes. In particular, the one-dimensional skewed finite difference operations should then be considered to act on surface-averaged values of the numerical solution. The total induced filter will then consist of a combination of filters due to the upwind scheme and filters associated with the surface averaging.

In the next section we return to the decomposition (7) of the computational stress tensor ξ and compare the magnitude of the turbulent stress tensor τ with the additional high-pass

contribution $\mathcal{H}(\bar{u}^2)$. We specifically concentrate on the influence of the subgrid resolution and the order of the discretization method.

IV. MAGNITUDE OF NUMERICAL HIGH-PASS CONTRIBUTIONS

In this section we will consider the computational stress tensor ξ in (7) associated with central and upwind differencing methods. For individual Fourier modes the expressions for τ and $\mathcal{H}(\bar{u}^2)$ can be made explicit, which is used in order to compare their dynamic relevance.

In the sequel we assume $u = e^{iKx}$ and adopt a symmetric top-hat filter as a basic large-eddy filter, with filter width Δ and characteristic function $\Gamma(K\Delta/2)$; i.e., $\bar{u} = \Gamma(K\Delta/2)u$. After some calculation, we obtain for the turbulent stress:

$$\tau = \overline{u^2} - \bar{u}^2 = e^{2iKx} \left[\Gamma(K\Delta) - \Gamma^2\left(\frac{K\Delta}{2}\right) \right]. \quad (49)$$

For a central discretization of order $2n$, the high-pass filter effect may be written as

$$\begin{aligned} \mathcal{H}(\bar{u}^2) &= \Gamma^2\left(\frac{K\Delta}{2}\right) \mathcal{H}(e^{2iKx}) \\ &= e^{2iKx} \left[\Gamma^2\left(\frac{K\Delta}{2}\right) [1 - \mathcal{G}_{-n,n}(2Kh)] \right]. \end{aligned} \quad (50)$$

The dynamic importance of these terms is represented most directly by considering the fluxes $\partial_x \tau = iA_x e^{2iKx}$ and $\partial_x \mathcal{H}(\bar{u}^2) = iA_x \mathcal{H}(e^{2iKx})$. The amplitudes of these fluxes, multiplied with Δ , are, respectively, given by

FIG. 4. The product of the filter width Δ and the amplitude of the fluxes due to the turbulent stress tensor τ ($A_\tau\Delta$: solid) and due to the high-pass filtering of $\bar{u}^2$ ($A_H\Delta$) for subfilter resolutions $r=1$ (dashed), $r=2$ (dash-dotted), and $r=4$ ($\circ$), and second-order (thin lines) or fourth-order (thick lines) central differencing. For ease of comparison, $-A_\tau\Delta$ was plotted.

$$A_\tau\Delta = 2K\Delta \left[\Gamma(K\Delta) - \Gamma^2\left(\frac{K\Delta}{2}\right) \right],$$

$$A_H\Delta = 2K\Delta\Gamma^2\left(\frac{K\Delta}{2}\right) \left[1 - \mathcal{G}_{-n,n}\left(\frac{2K\Delta}{r}\right) \right],$$
(51)

where we used the subfilter resolution $r=\Delta/h$ to express the amplitudes entirely as functions of $K\Delta$.

We compare the flux amplitudes in Fig. 4 as a function of $K\Delta$ at different subfilter resolutions $r=\Delta/h$. The amplitudes are seen to depend strongly on r . As $r=1$, we notice that for a wide range of wave numbers the amplitude of the high-pass filter contribution is larger than that of the flux due to the turbulent stress. This arises for both the second- and the fourth-order accurate central discretization. If the subfilter resolution is increased to $r=2$ the numerical high-pass filter terms decrease considerably and become about equal to or smaller than the turbulent stress flux. Only if we increase to $r=4$ we notice that the high-pass filter contribution is considerably smaller than the turbulent stress flux. The reduction of the high-pass filter contribution is strongest for the higher order discretization method. This is consistent with observations in Refs. 8 and 9, which were based on actual large-eddy simulations of homogeneous turbulence and turbulent mixing.

In case a general skewed finite differencing method is adopted, the flux due to the high-pass filter contribution may be expressed as

$$\partial_x \mathcal{H}(\bar{u}^2) = \partial_x [\bar{u}^2 - \mathcal{L}_{-n,m}(\bar{u}^2)] = ie^{2iKx} \{ \alpha_{-n,m} + i\beta_{-n,m} \},$$
(52)

where

$$\alpha_{-n,m} = 2k\Gamma^2\left(\frac{K\Delta}{2}\right) \left[1 - \mathcal{G}_{-n,m}\left(\frac{2K\Delta}{r}\right) \right],$$

$$\beta_{-n,m} = 2k\Gamma^2\left(\frac{K\Delta}{2}\right) \mathcal{I}_{-n,m}\left(\frac{2K\Delta}{r}\right).$$
(53)

In the symmetric case $m=n$, we observe that $\alpha_{-n,n}$ coincides with A_H as introduced in (51), and $\beta_{-n,n}=0$. In Fig. 5 we represented the amplitudes $\alpha_{0,n}$ and $\beta_{0,n}$ corresponding to

FIG. 5. Product of filter width Δ and the amplitude of the high-pass filter flux due to first-order (a) and second-order (b) forward discretization. The thin solid line corresponds to $-A_\tau\Delta$ to represent the amplitude of $\partial_x \tau$. The thin lines display $\alpha_{0,n}\Delta$ and the thick lines denote $\beta_{0,n}\Delta$ at $r=1$ (dashed), $r=2$ (dash-dotted), and $r=4$ ($\circ$).

first- and second-order forward differencing. The contributions represented by $\beta_{0,n}$ are solely due to the skewness of the stencil, while the equivalent of the $\alpha_{0,n}$ component is also observed in (51). Generally, for $r=1-2$, the amplitudes $\alpha_{0,n}$ and $\beta_{0,n}$ are quite comparable to the magnitude of $\partial_x \tau$. A strong reduction in the amplitudes $\alpha_{0,n}$ arises with increasing subfilter resolution. The reduction of the contributions represented by $\beta_{0,n}$ with increasing r is less pronounced. Moreover, we notice that both $\alpha_{0,n}$ and $\beta_{0,n}$ assume comparable values, which is an indication of significant numerical phase-shifts in the computational fluxes.

V. CONCLUDING REMARKS

In this paper we considered the contributions to the large-eddy closure problem arising from the spatial discretization. In case the subfilter resolution is coarse, the particular discretization scheme that is adopted in the computational model, has a large dynamic effect relative to the flux due to the turbulent stress. The difference between the actual computational stress tensor ξ and the turbulent stress tensor τ may be expressed most directly in terms of the *modified* equation. An additional flux arises in the modified equation which incorporates the numerical high-pass filter applied to $\bar{u}^2$. The analysis suggests that considerable improvements of practical large-eddy simulation may be achieved in case the closure problem in the modified equation is made to explicitly account for the coarseness as well as the type of discretization.

The induced numerical filter corresponding to central and skewed finite differencing was explicitly calculated. It was shown that higher-order discretization schemes induce higher order filters that may be expressed as linear combinations of the top-hat filter. These induced filters either affect only the amplitude (in case of central methods) or both the amplitude and the phase (in case of skewed methods) of individual Fourier modes. The dynamic importance of the high-pass filter contributions relative to the turbulent stress tensor depends considerably on the subfilter resolution. For values as low as $r=1-2$, the induced high-pass filter contribution is comparable to or even larger than the term that requires closure in large-eddy simulation. This was observed earlier in a *posteriori* analysis of turbulent mixing.¹⁵ In case $r \geq 4$ it appears that the dynamic consequences of the high-pass filter term can safely be neglected. This reduction of the numerical influences with increasing r is stronger in case the order of accuracy of the spatial discretization is higher. This underlines and further quantifies the observations reported in Refs. 8 and 9, in which complete database approaches to error dynamics in large-eddy simulation of homogeneous turbulence and turbulent mixing were presented.

The presented analysis of the filter induced by the spatial discretization method, and the quantitative comparison between the exact turbulent stress tensor and the implicit filtering contribution of different discretization schemes, is limited to considerations of single Fourier modes. An analysis of the possible nonlinear interference between numerical discretization and large-eddy modeling was pioneered in Ref. 6. Such nonlinear analysis addresses mainly *a priori* aspects of

the interacting error behavior within the joint-normal approximation for turbulent velocity fields. In order to extend these studies to include *a posteriori* aspects of the interacting discretization and subgrid modeling errors, the confrontation with actual large-eddy simulation of turbulent flow forms a relevant extension.⁸ Such a simulation approach allows one to fully investigate possible nonlinear accumulation of the effects of the different error contributions, as the turbulent flow develops in time. It may put the current study of the error behavior of different higher-order discretization methods in its proper perspective. For this purpose, an extensive simulation study of canonical flows such as decaying homogeneous turbulence, turbulent mixing layers, and turbulent flow in a channel can be undertaken along lines developed in Refs. 9 and 16. This is the subject of ongoing research. The interpretation of the results of such a numerical study can benefit from the modified equation analysis and the distinction made between the numerical turbulent stress tensor ξ and the more traditional turbulent stress tensor τ , as discussed in this paper.

For an explicit time-stepping method and a uniform computational grid, every doubling of the subfilter resolution r at fixed filter width Δ corresponds to about a factor of 16 increase in computational effort.³² This makes the near-grid-independency requirement $r \geq 4$ quite unattainable in practical applications of large-eddy simulation. The analysis presented in this paper indicates that one should fully incorporate the discretization effects into the modeling of the subfilter scales. Several possible strategies may be investigated in this respect. At one extreme of the spectrum of large-eddy methods, MILES¹⁸ relies entirely on the dissipative nature of the adopted spatial discretization methods, and no explicit model for the turbulent stress tensor τ_{ij} is introduced. Alternatively, the decomposition (7) presented in this paper advocates separate modeling of this stress tensor, next to explicit incorporation of the numerical high-pass filter contributions. This route offers more independent control over the various sources of error in large-eddy simulation. Since the computational turbulent stress tensor ξ_{ij} can be shown to obey Germano's identity,³³ much like τ_{ij} does, a bridge between MILES and more traditional LES can be conceived. Such an approach would, on the one hand, make the total subfilter modeling sensitive to the adopted numerical method and discrete representation, while, simultaneously, retain a close connection with rigorous mathematical properties of the filtered governing equations. This modeling strategy is the subject of current research.

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