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BRIEF COMMUNICATIONS

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Local spectrum of commutation error in large eddy simulations

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In this Brief Communication we present a new mathematical tool, which we call *local spectrum* analysis, that can be used to obtain information about local spectral content of the commutation error in large eddy simulations and its dependence on the filter shape and the non-uniformity of the filter width. To illustrate these theoretical findings, the local commutation spectrum analysis is applied to the results of 256^3 direct numerical simulation of forced homogeneous turbulence at $\mathrm{Re}_\lambda = 168$. The results confirm strong dependence of the spectral content of the commutation error on the filter shape: the spectrum is wide for smooth filters like Gaussian, while for filters, that are close to the sharp cut-off, the spectral content is localized. It is also demonstrated that the amplitude of the commutation error is linearly proportional to the filter width stretching factor. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1637605]

In large eddy simulation (LES) of turbulent flows the dynamics of the large scale structures are computed, while the effect of the small scale turbulence is modeled. The differential equations describing the space–time evolution of the large scale structures are formally derived by applying a low-pass filter with non-uniform filter width to the Navier–Stokes equations. For an incompressible flow the filtered Navier–Stokes equations, written in terms of filtered quantities, take the following form:

$$\frac{\partial \bar{u}_i}{\partial x_i} = -\left[\frac{\partial u_i}{\partial x_i}\right], \tag{1}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \overline{u_i u_j}}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \left[\frac{\partial u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{1}{\mathrm{Re}}\frac{\partial^2 u_i}{\partial x_j \partial x_j}\right], \tag{2}$$

where the square bracket denotes the commutation operator given by

$$\left[\frac{\partial F}{\partial x_i}\right] = \overline{\frac{\partial F}{\partial x_i}} - \frac{\partial \bar{F}}{\partial x_i}. \tag{3}$$

The filtered convective term $\overline{u_i u_j}$ is unknown in LES and is typically decomposed into the convective term $\bar{u}_i \bar{u}_j$ that can be computed and the remainder, called sub-grid scale (SGS) stress, which should be modeled

$$\overline{u_i u_j} = \bar{u}_i \bar{u}_j - \underbrace{(\bar{u}_i \bar{u}_j - \overline{u_i u_j})}_{\tau_{ij}}. \tag{4}$$

In order to derive LES equations from Eqs. (1), (2), and (4) it is commonly assumed that the differentiation and filtering operations commute. With this assumption we obtain the classical LES equations

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{5}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j}. \tag{6}$$

Commutation is generally satisfied if the filter has a constant width. However, this assumption is invalid if the filter width is not uniform—as in the case of wall-bounded flows—unless special filter operators are constructed. Recently a new class of *commutative* filters for both structured[1] and unstructured[2,3] grids has been developed. With these filters the differentiation and filtering operations commute to an *a priori* specified order of filter width. The desired commutation error is achieved by constructing filters in such a way that the filter moments $M^{ijk}(\mathbf{x}) = \oint_D y_1^i y_2^j y_3^k \mathcal{G}(\mathbf{y};\mathbf{x}) d^3\mathbf{y}$ satisfy the following constraints:

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$$M^{ijk}(\mathbf{x})=\begin{cases}1 & i,j,k=0,\\ 0 & 0<i+j+k<n,\end{cases}\tag{7}$$

where $\mathbf{x}=(x_1,x_2,x_3)$ explicitly denotes the location of the filter, n is the number of vanishing moments, and $\mathcal{G}(\mathbf{y};\mathbf{x})$ is the location dependent three-dimensional filter function that defines the filtering operation as follows:

$$\bar{\phi}(\mathbf{x})=\oint_{\mathbf{D}}\mathcal{G}(\mathbf{y};\mathbf{x})\phi(\mathbf{y})d^3\mathbf{y}.\tag{8}$$

In this case it can be shown (see Refs. 1, 2, and 3) that for a smoothly varying filter width, the local commutation error in three dimensions is given by

$$\left[\frac{\partial\phi}{\partial x_1}\right]=O(\Delta_1^i(\mathbf{x})\Delta_2^j(\mathbf{x})\Delta_3^k(\mathbf{x})),\quad i+j+k=n.\tag{9}$$

Leading order commutation error analysis described above can be viewed as a practical tool for constructing discrete filters that commute with finite difference operators to an *a priori* specified order of filter width. However, the leading order error analysis by itself is not sufficient to guarantee that the commutation error is negligible compared to the subgrid scale stress, since it does not use any information about spectral content of the analyzed signal.[4,5] Due to the presence of significant energy in the high frequency portion of the LES spectrum, the commutation error could be considerable and in some cases even comparable with the subgrid scale stresses. In addition, the application of the standard or windowed Fourier transform for the analysis of the commutation error will result in a spectrum that does not differentiate between the different effects that influence it, namely the filter shape, filter width, and its spatial variation. Furthermore, the spectrum will be global and will not contain any local information of spatial variation in the spectral content of the commutation error.

The objective of this Brief Communication is to present a novel mathematical tool that can be used to analyze the local spectral content of the commutation error (hereafter referred as the *local spectrum* of the commutation error) and its dependence on the filter shape and the non-uniformity of the filter width.

We begin by introducing the *local spectrum* analysis in one-dimensional space and then extend it to three spatial dimensions. Let us consider a one-dimensional filter of constant shape but variable width. The continuous filtering operation can be written as

$$\bar{\phi}(x)=\frac{1}{\Delta(x)}\int_{-\infty}^{\infty}G\left(\frac{x-y}{\Delta(x)}\right)\phi(y)dy,\tag{10}$$

where, in contrast to Eq. (8), the filter shape is fixed throughout the domain, while the filter width changes as a function of position. Note that the filter can be either symmetric or asymmetric. Substituting the Fourier integral

$$\phi(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\hat{\phi}(k)e^{ikx}dk\tag{11}$$

into Eq. (10), changing the order of integration, and integrating the resulting equation with respect to y we obtain

$$\bar{\phi}(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\{\hat{G}(\Delta(x)k)\hat{\phi}(k)\}e^{ikx}dk,\tag{12}$$

where $\hat{G}(k)$ is the Fourier transform of the filter function given by

$$\hat{G}(k)=\int_{-\infty}^{\infty}G(\xi)e^{-ik\xi}d\xi.\tag{13}$$

Now comparing Eqs. (11) and (12) we can see that the structure of the equations is the same, except that the term in the curly brackets in Eq. (12) has implicit spatial dependence. Thus, the *local* Fourier transform of the filtered quantity $\bar{\phi}$ can be defined as

$$\hat{\bar{\phi}}(k;x)=\hat{G}(\Delta(x)k)\hat{\phi}(k).\tag{14}$$

Note that in order to calculate $\bar{\phi}$ at a specific location, x_0, we only need to know the *local spectrum* $\hat{\bar{\phi}}(k;x_0)$. Now the meaning of the *local* Fourier transform is clear: it refers to the location in space, where the transform is taken, and gives the information about the spectral content of the commutation error. Also it reflects the fact that the filter width is a function of location. Performing analogous analysis for the commutation error it can be shown that

$$\left[\frac{d\phi}{dx}\right](x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left\{\frac{1}{\Delta(x)}\frac{d(\Delta(x))}{dx}\hat{K}(k_\Delta)\hat{\phi}(k)\right\}e^{ikx}dk,\tag{15}$$

where $k_\Delta=\Delta(x)k$ and the transfer function $\hat{K}(k)$ is defined by

$$\hat{K}(k)=-k\frac{d\hat{G}(k)}{dk}.\tag{16}$$

Analogously to Eq. (14), the *local* one-dimensional spectrum of the commutation error is defined as

$$\left[\widehat{\frac{d\phi}{dx}}\right](k;x)=\frac{1}{\Delta(x)}\frac{d(\Delta(x))}{dx}\hat{K}(k_\Delta)\hat{\phi}(k).\tag{17}$$

Now the effect of filtering is clearly seen: filter width stretching factor, $[1/\Delta(x)][d(\Delta(x))/dx]$, affects the amplitude of the commutation error, while the filter shape and width affect the local spectral content. The effect of the filter shape on the spectrum of commutation error is demonstrated in Fig. 1, where transfer functions $\hat{G}(k_\Delta)$ and $\hat{K}(k_\Delta)$ are shown for a variety of filters. The wavenumber k_Δ^c, which effectively defines the filter width,[6] is marked by a dashed vertical line. It is important to note that the closer the filter to the sharp cut-off, the more localized in wavenumber space the spectral content of the commutation error. Also note that the commutation error is exactly zero, when the width of the filter is constant throughout the domain.

The one-dimensional analysis can be easily extended to three spatial dimensions. In particular, it can be shown that for three-dimensional filters of constant shape and variable width the commutation error is given by

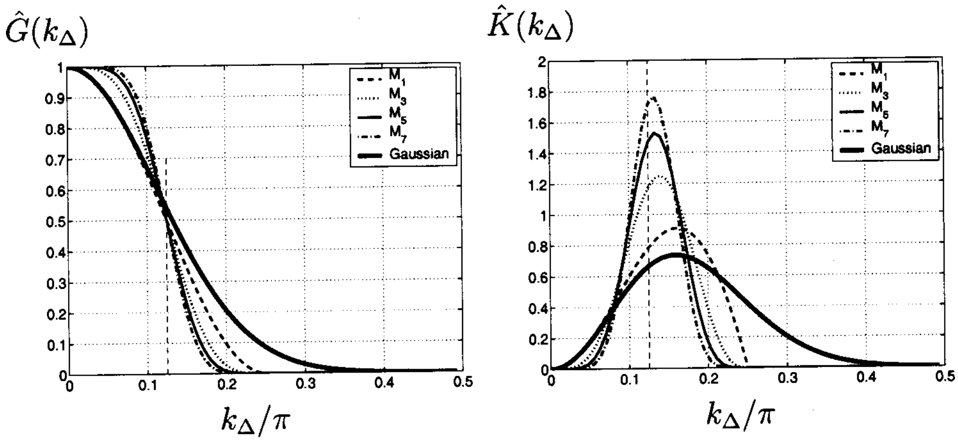

FIG. 1. Transfer functions $\hat{G}(k_\Delta)$ and $\hat{K}(k_\Delta)$ for a variety of filters. M_n denotes the discrete filter with n vanishing moments.

$$\left[\frac{\partial \phi}{\partial x_i}\right](\mathbf{x}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{\sum_{l=1}^{3}\frac{1}{\Delta_l(\mathbf{x})}\frac{\partial(\Delta_l(\mathbf{x}))}{\partial x_i}\times\hat{K}_l(\mathbf{k}_\Delta)\hat{\phi}(\mathbf{k})\right\}e^{i\mathbf{k}\mathbf{x}}d^3\mathbf{k}, \tag{18}$$

where $\Delta_i(\mathbf{x})$ is the filter width in the x_i direction, $\mathbf{k}=(k_1,k_2,k_3)^T$ and $\mathbf{k}_\Delta=(\Delta_1(\mathbf{x})k_1,\Delta_2(\mathbf{x})k_2,\Delta_3(\mathbf{x})k_3)^T$ are three-dimensional wave vectors, $\hat{\phi}(\mathbf{k})$ is the Fourier transform of function $\phi(\mathbf{x})$, $\hat{G}(\mathbf{k})$ is the Fourier transform of the filter function, and the transfer function $\hat{K}_l(\mathbf{k})$ is defined by

$$\hat{K}_l(\mathbf{k}) = -k_l\frac{\partial \hat{G}(\mathbf{k})}{\partial k_l}. \tag{19}$$

It is important to note that the *local spectrum* analysis can be applied in a more general setting, when the global Fourier transform does not exist due to the presence of boundaries. In this case, the global Fourier transform can be simply replaced by the windowed Fourier transform and all conclusions drawn in the paper will be still valid. The only limitation is that the support of the Fourier window should be within the physical domain. Also note that the windowed Fourier analysis is not applicable in the immediate vicinity of solid boundaries. However, close to the boundaries, spectral content of the LES is limited to low frequencies. Thus, in the immediate vicinity of the boundary the leading order error analysis could provide reliable information about the commutation error.

Another important point that we want to elaborate on, is a physical interpretation of the *local spectrum* concept. We use the word "local" to emphasize the fact that the *local spectrum* analysis provides the information about the spectral content of the commutation error, which is associated with a particular point in space, where the filter shape, width, and filter width stretching factor are known. In general, when this analysis is applied to an inhomogeneous case, the windowed Fourier energy spectrum changes from location to location. However, if *local spectrum* analysis is applied to the case, where the global spectrum exists and the filter width varies only in one spatial direction, then the only two parameters that affect the spectral content of the commutation error are the filter width and filter width stretching factor. In this case for any two points that have the same filter width, the local spectral content of the commutation error will differ only in the amplitude that is determined by the filter width stretching factor. Thus in this case, the location for the *local spectrum* analysis does not need to be explicitly specified.

To demonstrate the effect of commutation error in LES, we apply the local commutation error analysis to the results of 256^3 direct numerical simulation (DNS) of forced homogeneous turbulence[7] at $\mathrm{Re}_\lambda=168$. It should be emphasized that the homogeneous turbulence field is used for illustration purposes only and, as was mentioned earlier, the analysis can be applied in a more general setting using the windowed Fourier transform. Figure 2 shows the *local* one-dimensional spectrum of commutation error for the Gaussian and the discrete M_7 filter (see Fig. 1). These two filters are chosen because the Gaussian filter is smooth, while the M_7 filter is close to the sharp cut-off filter. The wavenumber k_1^c, which effectively defines the filter width[6] in the x_1 direction, is

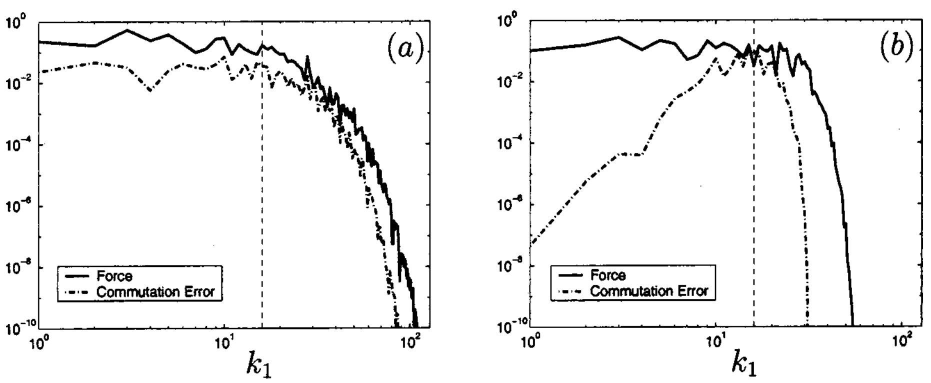

FIG. 2. Global one-dimensional spectrum of the exact SGS force, $\partial\tau_{11}/\partial x_1$, and *local* one-dimensional spectrum of the commutation error, $[\partial u_1^2/\partial x_1]$, for forced isotropic turbulence at $\mathrm{Re}_\lambda=168$ for (a) Gaussian and (b) M_7 filters.

marked by a dashed vertical line. Note that the filter width, Δ_1, that was used in these calculations can be easily extracted from k_Δ^c and k_1^c. Also note that at any given point in space the filter width and the stretching factors are sufficient for the calculation of the *local spectrum* of commutation error [see Eq. (18)]. Consequently, the actual filter width distribution is not required for the calculation of the *local spectrum* of commutation error. Note that the *local spectrum* of the commutation error shown in Fig. 2 assumes a unity filter width stretching factor. In contrast, the local windowed Fourier spectrum for the SGS force, $\partial \tau_{11} / \partial x_1$, at any given point requires knowledge of the actual filter width distribution. However, the global spectrum of the exact SGS force is a good approximation for the slowly varying filter width case. For that reason the global one-dimensional spectrum of the exact SGS force is also shown in Fig. 2 for reference. The exact SGS force is obtained by filtering the DNS data using Gaussian and M_7 filters (see Fig. 1) with the same filter width that is used in the calculation of the *local spectrum* of the commutation error. The results confirm strong dependence of the spectrum of commutation error on the filter shape: the spectrum is global for smooth filters like Gaussian, while for filters, that are close to the sharp cut-off, the spectrum is localized. In addition, the *local spectrum* analysis confirms that in order for the commutation error to be negligible compared to the SGS force, the filter width stretching factor should be considerably below unity.

In conclusion we want to emphasize that the *local spectrum* analysis, proposed in this Brief Communication, provides new theoretical insights on the spectral content of the commutation error. It gives a LES practitioner the guidelines on how to decrease the effect of the commutation error and provides a new way to look at the spectral content of the commutation error.

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