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The Basic Equations for the Large Eddy Simulation of Turbulent Flows in Complex Geometry

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The equations for large eddy simulation (LES) of turbulent flows are derived by applying a "filtering" operation to the Navier–Stokes equations. LES of inhomogeneous turbulent flows requires the use of filters with variable filter width. The use of such filters invalidates the standard derivation of the basic equations for the filtered fields since the filtering operation in general does not commute with the operation of differentiation. In this paper an alternate definition of the filtering operation based on the mapping function of the nonuniform grid is introduced. It is shown that with this modified definition the filtering and differentiation operations commute up to an error which is second order in the filter width. It is also shown that the commutation error can be expressed in terms of the filtered field and its derivatives as an asymptotic series in the square of the filter width. These results are then applied to the Navier–Stokes equations to derive the basic equations satisfied by the filtered fields. © 1995 Academic Press, Inc.

1. INTRODUCTION

Application of the method of LES to a turbulent flow consists of three separate steps. First, a filtering operation is performed on the Navier–Stokes equations to remove the small spatial scales. The resulting equations that describe the space–time evolution of the "large eddies" contain the subgrid scale (sgs) stress tensor that describes the effect of the unresolved small scales on the resolved scales. In principle, the sgs stress depends on the precise definition of the filtering operation and the parameters characterizing it. The second step is the replacement of the sgs stress (which is unknown, since it depends on the unresolved scales) by a "model." The "model" may be any expression that can be calculated from the resolved scales and may or may not contain some adjustable parameters. The final step is the numerical simulation of the resulting "closed" equations for the large scale fields on a grid small enough to resolve the smallest of the large eddies, but still much larger than the fine scale structures at the Kolmogorov length.

In this paper, we will focus our attention on the first step, that is, the derivation of the basic equations describing the evolution of the large eddies of a turbulent inhomogeneous flow. This should not be confused with issues such as finite differencing errors or the best choice of computational grids which are part of the third stage mentioned above. The only connection between the derivation of the large eddy equations presented in this paper and choice of grids in numerical simulations is that the local grid spacing must be of the same order as the local filter width to ensure that the grid is just fine enough to resolve the filtered fields. In practice it is convenient to first find an appropriate computational grid and then define a filtering operation consistent with it.

In dividing a turbulent flow field into "large" and "small" eddies one presumes that a cut-off length δ can be sensibly chosen such that all fluctuations on a scale larger than δ are "large eddies" and the remainder constitute the "small scale" fluctuations. Typically, δ would be a length scale characterizing the smallest structures of interest in the flow. In an inhomogeneous flow, the "sensible choice" for δ may vary significantly over the flow domain. For example, in a wall-bounded turbulent flow, most statistical averages of interest vary much more rapidly with position near the wall than far away from it. Further, there are dynamically important organized structures near the wall on a scale much smaller than the boundary layer thickness. Therefore, the minimum size of eddies that need to be resolved is smaller near the wall. In general, for the LES of inhomogeneous flows we must consider the width of the filtering kernel δ to be a function of position.

If a filtering operation with a nonuniform filter width is performed on the Navier–Stokes equations, one does not in general get the standard large eddy equations. The complication is caused by the fact that a filtering operation with a nonuniform filter width in general does not commute with the operation of differentiation. The purpose of this paper is to address this specific problem. In the next section it is shown that a variable width filter can be derived from a given fixed-width filter by means of a nonlinear mapping procedure, and this definition is adopted for future work by virtue of its desirable properties, discussed in the rest of this paper. It is shown in Section 3 that, in addition to being intuitively appealing, the filtering operation so defined has the property that the commutation error goes to zero with the filter width. In Section 4 we show how the commutation error is distributed over all possible wave numbers. In Section 5, we show how the lack of commutation

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between the filtering and differentiation operations can be corrected for at successive orders in the filter width. The extra terms introduced in the large eddy equations as a result of these corrections have intuitive physical interpretations which are discussed in Section 6 with the help of a simple model equation. The results of these investigations in one dimension are extended to general three-dimensional flows in Section 7. The higher order corrections needed to account for the commutation error raise the spatial order of the differential equations. Therefore, additional boundary conditions are required in order to uniquely determine the solution. This issue is discussed in Section 8. The preceding ideas are brought together in Section 9 to derive the large eddy equations for a general inhomogeneous turbulent flow. A perturbative method for computing the filtered fields to any order is also presented. Conclusions are summarized in Section 10.

2. NONUNIFORM FILTERING IN ONE SPACE DIMENSION (DEFINITION)

Consider a field $\phi(\xi)$ defined in the domain $(-\infty, +\infty)$. A filtering operation with a constant filter width Δ is defined by [2]

$$\overline{\phi}(\xi) = \frac{1}{\Delta}\int_{-\infty}^{+\infty} G\left(\frac{\xi-\eta}{\Delta}\right)\phi(\eta)\,d\eta, \qquad (2.1)$$

where G is any function with domain $(-\infty, +\infty)$ and endowed with the following properties:

(i) $G(-\xi) = G(\xi)$

(ii) $\int_{-\infty}^{+\infty} G(\xi)\,d\xi = 1$

(iii) $G(\xi) \to 0$ as $|\xi| \to \infty$ sufficiently fast so that all moments

$$\int_{-\infty}^{+\infty} G(\xi)\xi^n\,d\xi$$

($n \geq 0$) exist.

(iv) $G(\xi)$ is localized (in some suitably defined sense) in $(-\frac{1}{2}, +\frac{1}{2})$.

Some examples of possible filter functions are the "top-hat" filter,

$$G(\xi) = \begin{cases} 1, & \text{if } |\xi| \leq \frac{1}{2}, \\ 0, & \text{otherwise}, \end{cases} \qquad (2.2)$$

and the "Gaussian" filter,

$$G(\xi) = \sqrt{\frac{2}{\pi}}\exp(-2\xi^2). \qquad (2.3)$$

(For a discussion of the various types of filters used in LES, see [1].)

In situations where the domain might be finite or semi-infinite and a variable filter width is desirable, the definition (2.1) can have many possible generalizations. For example, a generalization of (2.1) when G is the top-hat filter might be

$$\overline{\phi}(\xi) = \frac{1}{(\Delta_+(\xi) + \Delta_-(\xi))}\int_{\xi-\Delta_-(\xi)}^{\xi+\Delta_+(\xi)} \phi(\eta)\,d\eta \qquad (2.4)$$

where $\Delta_+(\xi)$ and $\Delta_-(\xi)$ are positive functions and $\Delta_+(\xi) + \Delta_-(\xi)$ is the effective filter width at location "ξ". For a finite or semi-infinite domain, $\Delta_+(\xi)$ and $\Delta_-(\xi)$ must go to zero at the boundaries sufficiently rapidly so that $(\xi - \Delta_-(\xi), \xi + \Delta_+(\xi))$ is always in the domain of ϕ. It may be shown [5] that with the definition (2.4),

$$\begin{aligned} \overline{\frac{d\phi}{d\xi}} - \frac{d\overline{\phi}}{d\xi} &= \frac{(d/d\xi)(\Delta_+(\xi) + \Delta_-(\xi))}{\Delta_+(\xi) + \Delta_-(\xi)}\overline{\phi} \\ &- \frac{1}{(\Delta_+ + \Delta_-)}\left[\phi(\xi + \Delta_+)\frac{d\Delta_+}{d\xi}\right. \qquad (2.5) \\ &\left. + \phi(\xi - \Delta_-)\frac{d\Delta_-}{d\xi}\right]. \end{aligned}$$

Thus,

$$\left(\overline{\frac{d\phi}{d\xi}}\right) \neq \frac{d\overline{\phi}}{d\xi}. \qquad (2.6)$$

One would like to believe that the right-hand side of (2.5) would be small for some reasonable class of nonuniform filters but this has never been conclusively demonstrated. This lack of commutativity between filtering and differentiation causes every spatial derivative operator in the Navier–Stokes equations to generate terms that cannot be expressed solely in terms of the filtered fields. Therefore, a "closure problem" is introduced not only for the nonlinear terms but for the linear terms as well. To remedy this situation we first propose an alternate definition for the filtering operation that is more general than (2.4).

Let ϕ be some field defined in a finite or infinite domain $[a, b]$. Any nonuniform grid in the domain $a \leq x \leq b$ can be mapped to a uniform grid of spacing Δ in the domain $[-\infty, +\infty]$ by means of some mapping function

$$\xi = f(x). \qquad (2.7)$$

Here $f(x)$ is a monotonic differentiable function such that

$$f(a) = -\infty, \qquad (2.8)$$

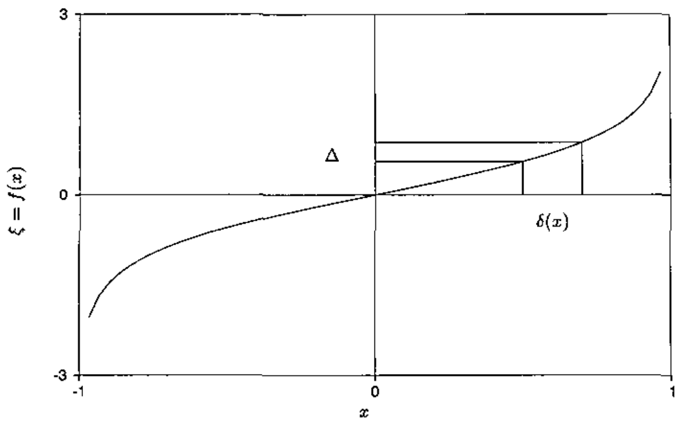

FIG. 1. The space x, with variable filter width $\delta(x)$, is shown mapped into a space ξ, with constant filter width Δ, by the "tan-hyperbolic map" $f(x) = \tanh^{-1}x$.

$$f(b) = +\infty. \tag{2.9}$$

The nonuniform grid spacing $\delta(x)$ is clearly given by

$$\delta(x) = \frac{\Delta}{f'(x)} \tag{2.10}$$

(see Fig. 1). Clearly, if a (or b) is finite, (2.8)–(2.9) require $f'(a)$ (or $f'(b)$) to be infinite so that $\delta(a)$ (or $\delta(b)$) $= 0$. Thus, the filtering kernel becomes a Dirac delta function at finite boundaries.

The filtering operation is defined as follows. Given an arbitrary function $\psi(x)$ we first make a change of variables to ξ to obtain the new function $\phi(\xi) = \psi(f^{-1}(\xi))$. The function $\phi(\xi)$ is then filtered using the usual definition (2.1) appropriate for filtering on a uniform grid. Finally, we transform back to the variable x. Thus,

$$\overline{\psi}(x) \equiv \overline{\phi}(\xi) = \frac{1}{\Delta}\int_{-\infty}^{+\infty} G\left(\frac{f(x) - \eta}{\Delta}\right)\phi(\eta)\, d\eta \tag{2.11}$$

or, on using (2.7), we have

$$\overline{\psi}(x) = \frac{1}{\Delta}\int_a^b G\left(\frac{f(x) - f(y)}{\Delta}\right)\psi(y) f'(y)\, dy. \tag{2.12}$$

Equation (2.11) or, equivalently, (2.12) is the definition we shall adopt for the filtering operation with a nonuniform filter width. For reasons that will become apparent in the next section, we will call this the Second-Order Commuting Filter (SOCF). It should be noted that the definiton (2.4) used by Moin *et al.* is quite different from what one would get on substituting the expression (2.2) for the top-hat filter into (2.12).

Example. In channel flow one often uses the "tanhyperbolic grid" [3],

$$f(x) = \tanh^{-1}x, \tag{2.13}$$

where $+1 \geq x \geq -1$. ($x = \pm 1$ corresponds to the channel walls.) From Eq. (2.12), the filtering operation is defined as

$$\overline{\psi}(x) = \int_{-1}^{+1} \tilde{G}(x, y)\psi(y)\, dy, \tag{2.14}$$

where

$$\tilde{G}(x, y) = \frac{1}{\Delta} G\left(\frac{f(x) - f(y)}{\Delta}\right) f'(y) \tag{2.15}$$

with $f(x) = \tanh^{-1}x$. The function $\tilde{G}(x, y)$ is plotted in Fig. 2A when G is a top-hat filter and in Fig. 2B when G is a Gaussian filter. If the approximations $f(x) - f(y) \approx f'(x)(x - y)$ and $f'(y) \approx f'(x)$ for y near x are used in (2.15), we have, on using (2.10),

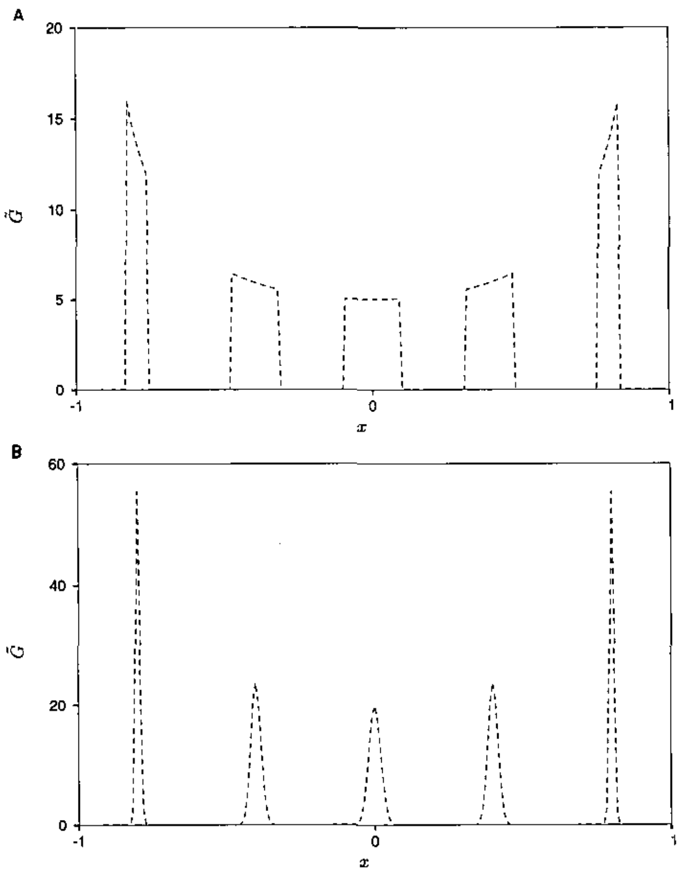

FIG. 2. The shape of the filter function $\tilde{G}$ (a) when G is a top-hat filter and (b) when G is a Gaussian filter.

$$\tilde{G}(x, y) \approx \frac{1}{\delta(x)} G\left(\frac{x-y}{\delta(x)}\right). \tag{2.16}$$

Thus, as a first approximation, the filtering kernel $\tilde{G}$ contracts in a self-similar manner on approaching a finite boundary (see Figs. 2A and 2B). However, the exact formula (2.15) has an additional higher order effect that causes the filter function $\tilde{G}$ to become asymmetric near the wall, giving more weight to points nearer the wall than further from it. The effect is most clearly seen in Fig. 2A.

3. CALCULATION OF THE COMMUTATION ERROR

On differentiating Eq. (2.12) with respect to x and performing an integration by parts, we obtain

$$\frac{d\bar{\psi}}{dx} = -\frac{f'(x)}{\Delta}\left[G\left(\frac{f(x)-f(y)}{\Delta}\right)\psi(y)\right]_{y=a}^{y=b} + \frac{1}{\Delta}\int_a^b G\left(\frac{f(x)-f(y)}{\Delta}\right) f'(x)\psi'(y)\,dy. \tag{3.1}$$

By virtue of Eqs. (2.8)–(2.9) and the condition $G(\pm\infty) = 0$, the boundary term vanishes. (Since ψ is a physical field, we assume that it remains bounded at the domain boundaries.) Thus, we have

$$\begin{aligned}\mathscr{C}[\psi] &\equiv \overline{\left(\frac{d\psi}{dx}\right)} - \frac{d\bar{\psi}}{dx} \\ &= \frac{1}{\Delta}\int_a^b G\left(\frac{f(x)-f(y)}{\Delta}\right)\psi'(y)f'(y) \\ &\quad\times\left[1-\frac{f'(x)}{f'(y)}\right]dy.\end{aligned} \tag{3.2}$$

It is convenient to introduce the new variable ζ such that y is expressed implicitly in terms of ζ through the equation

$$f(y) = f(x) + \Delta\zeta. \tag{3.3}$$

Equation (3.3) can be inverted by expressing y in a power series

$$y = y_0(\zeta) + \Delta y_1(\zeta) + \Delta^2 y_2(\zeta) + \cdots. \tag{3.4}$$

On substituting (3.4) in (3.3) and equating like powers of Δ, one obtains the expansion

$$y = x + \frac{\Delta\zeta}{f'} - \frac{\Delta^2 f''}{2f'^3}\zeta^2 + \cdots. \tag{3.5}$$

(*Note.* When the argument of any function is omitted we imply that the function is evaluated at "x".)

In terms of ζ, Eq. (3.2) may be written as

$$\mathscr{C}[\psi] = \int_{-\infty}^{+\infty} G(\zeta)\psi'(y)\left[1-\frac{f'(x)}{f'(y)}\right]d\zeta \tag{3.6}$$

where y is given by (3.5) (the limits of integration are obtained on using (2.8) and (2.9) in (3.3)). On expanding each of the factors in the integrand of (3.6) in Taylor series in Δ and collecting terms of the same order, we have

$$\mathscr{C}[\psi] = c_1\Delta + c_2\Delta^2 + \cdots, \tag{3.7}$$

where

$$c_1 = \frac{f''\psi'}{f'^2}\int_{-\infty}^{+\infty}\zeta G(\zeta)\,d\zeta \tag{3.8}$$

and

$$c_2 = \frac{2f'f''\psi'' + f'f'''\psi' - 3f''^2\psi'}{2f'^4}\int_{-\infty}^{+\infty}\zeta^2 G(\zeta)\,d\zeta. \tag{3.9}$$

Since $G(\zeta)$ is symmetric, $c_1 = 0$. Thus, the commutation error $\mathscr{C}[\psi] \sim O(\Delta^2)$.

In an LES the grid spacing is approximately equal to the "filter width" which is of order Δ. If a second-order numerical scheme is used to represent the derivatives, the finite-differencing error is then of the same order as the error due to the lack of commutativity of the differentiation and the filtering operations. Therefore, in an LES of an inhomogeneous turbulent flow using a second-order finite differencing scheme, the filtering operation can be considered to commute with the differentiation operation to within the accuracy of the numerical approximation.

4. SPECTRAL DISTRIBUTION OF THE COMMUTATION ERROR

Let us substitute

$$\psi = \hat{\psi}_k \exp(ikx) \tag{4.1}$$

and (3.5) in (3.6). Then,

$$\begin{aligned}\mathscr{C}[\psi] &= ik\psi\int_{-\infty}^{+\infty} G(\zeta)\left[1-\frac{f'(x)}{f'(x+\Delta\zeta/f'+\cdots)}\right] \\ &\quad\times\exp\left(ik\frac{\Delta\zeta}{f'}+\cdots\right)d\zeta.\end{aligned} \tag{4.2}$$

On expanding the integrand of (4.2) in a power series in Δ, we have

$$\frac{\mathscr{C}[\psi]}{\psi} = \mathscr{F}_0(k\Delta) + \Delta\mathscr{F}_1(k\Delta) + \cdots, \tag{4.3}$$

where $\mathscr{F}_0$, $\mathscr{F}_1$, ... contain Δ only in the combination $k\Delta$.

Now $\Delta \ll 1$ but $k\Delta$ may be as large as order one. Thus, $\Delta \ll k\Delta$ so that we may neglect all but the first term in (4.3) to obtain

$$\frac{\mathscr{C}[\psi]}{\psi} \simeq \mathscr{F}_0(k\Delta). \tag{4.4}$$

On evaluating $\mathscr{F}_0(k\Delta)$ from (4.2) we have

$$\frac{\mathscr{C}[\psi]}{\psi} = ik\,\Delta\frac{f''}{(f')^2}\mathscr{F}\left(\frac{k\Delta}{f'}\right), \tag{4.5}$$

where $\mathscr{F}$ is defined by

$$\mathscr{F}(x) = \int_{-\infty}^{+\infty} \zeta G(\zeta)\exp(ix\zeta)\,d\zeta. \tag{4.6}$$

Equation (4.5) can also be written as

$$\frac{\mathscr{C}[\psi]}{\psi} = -ik\delta\left(\frac{\delta'}{\delta}\right)\mathscr{F}(k\delta), \tag{4.7}$$

where δ is the local filter width as defined in (2.10). On expanding the exponential in (4.6) in a Taylor series, we see, by virtue of $G(\zeta)$ being symmetric, that $\mathscr{F}(k\delta) \sim k\delta$ so that $|\mathscr{C}[\psi]/\psi| \sim (k\delta)^2$ as shown in the last section.

Comparison with finite differencing errors is facilitated if the commutation error is expressed as a "modified wave-number." If $\mathscr{C}[\psi]$ were zero, we will have for the function (4.1) that

$$\frac{d\overline{\psi}}{dx} = \frac{\overline{d\psi}}{dx} = \overline{ik\psi} = ik\overline{\psi}. \tag{4.8}$$

Therefore, if we define a modified wave-number k' by

$$\frac{d\overline{\psi}}{dx} = ik'\overline{\psi}, \tag{4.9}$$

then the departure of k' from k is a measure of the commutation error. On making the change of variable (3.3) in (2.12), we obtain

$$\overline{\psi}(x) = \int_{-\infty}^{+\infty} G(\zeta)\psi(y)\,d\zeta. \tag{4.10}$$

On substituting (4.1) in (4.10) and on using the definition (4.9), we obtain

$$\frac{k'}{k} = \frac{\int_{-\infty}^{+\infty} G(\zeta)\exp(iky(x,\zeta))(\partial y(x,\zeta)/\partial x)\,d\zeta}{\int_{-\infty}^{+\infty} G(\zeta)\exp(iky(x,\zeta))\,d\zeta}, \tag{4.11}$$

where y has been expressed as a function of ζ by inverting (3.3) for each fixed value of x. Equation (4.11) is an exact result. A simplified asymptotic form is obtained upon substituting the expansion (3.5) in (4.11) and dropping all terms such as $\Delta(k\Delta)$, $\Delta^2(k\Delta)$, ..., since it was shown above that $\Delta \ll k\Delta$. Thus,

$$\frac{k'}{k} = 1 - \Delta\frac{f''}{f'^2}\frac{\int_{-\infty}^{+\infty}\zeta G(\zeta)\exp(ik\,\Delta\zeta/f')\,d\zeta}{\int_{-\infty}^{+\infty} G(\zeta)\exp(ik\,\Delta\zeta/f')\,d\zeta}. \tag{4.12}$$

Since $G(\zeta)$ is a symmetric function, (4.12) simplifies to

$$\frac{k'}{k} = 1 - i\Delta\frac{f''}{f'^2}\frac{\int_{-\infty}^{+\infty}\zeta G(\zeta)\sin(k\,\Delta\zeta/f')\,d\zeta}{\int_{-\infty}^{+\infty} G(\zeta)\cos(k\,\Delta\zeta/f')\,d\zeta}. \tag{4.13}$$

EXAMPLE. Let us consider the top-hat filter defined by (2.2) together with the tan-hyperbolic map $f(x) = \tanh^{-1}x$. For this map, Eq. (3.3) can be inverted to give

$$y = \frac{x + \tanh\Delta\zeta}{1 + x\tanh\Delta\zeta}. \tag{4.14}$$

On substituting (4.14) in (4.11), we obtain

$$\frac{k'}{k} = \frac{\int_{-\infty}^{+\infty}\exp(iky)G(\zeta)[(1-\tanh^2\Delta\zeta)/(1+x\tanh\Delta\zeta)^2]}{\int_{-\infty}^{+\infty}\exp(iky)G(\zeta)\,d\zeta}, \tag{4.15}$$

with y given by (4.14). As an illustrative example we consider a channel whose walls are at $x = 0$ and $x = 2\pi$ with 17 grid points in the spanwise direction. Thus, $\Delta = 2\pi/16$. The integral (4.15) can be evaluated numerically. The result is shown in Fig. 3. The modified wavenumber for the second-order central difference scheme is given by

$$\frac{k'}{k} = \frac{\sin(k\delta)}{k\delta}. \tag{4.16}$$

Equation (4.16) is also plotted in Fig. 3 for comparison. The asymptotic formula (4.13) can be evaluated analytically in the case of the tan-hyperbolic map and top-hat filter. A straightforward computation gives

$$k' = k + \frac{2ix}{(1-x^2)}\left[\frac{k\delta}{2}\cot\left(\frac{k\delta}{2}\right) - 1\right]. \tag{4.17}$$

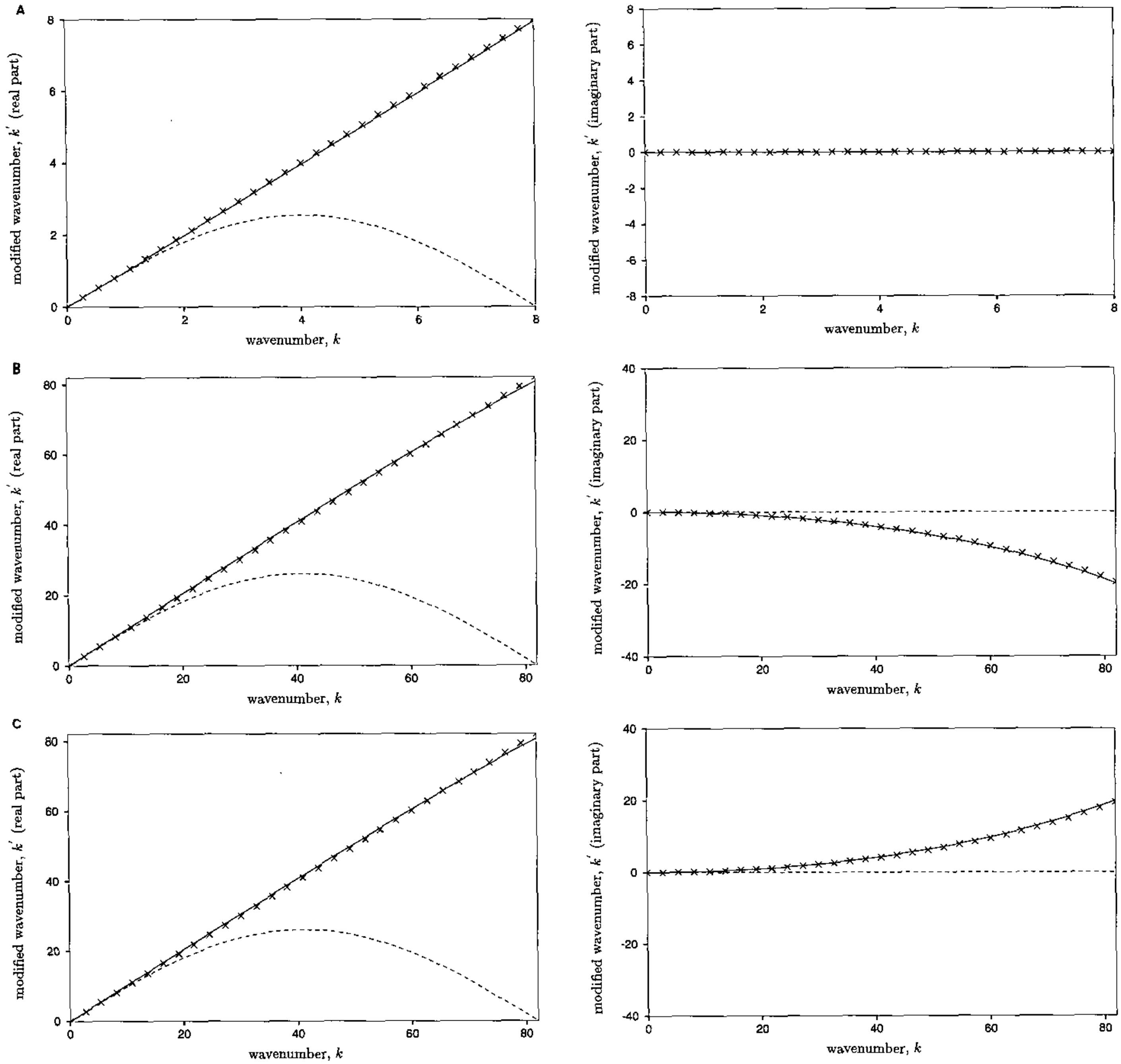

FIG. 3. (a) The real (left) and imaginary (right) parts of the commutation error (solid line) compared to the central differencing error (dotted line). The symbols "×" are the result of using the approximate formula (4.17). Here $\Delta = 2\pi/16$, $x = 0$ (channel center), and the maximum wavenumber is π/δ where δ is the local filter width. (b) Same as (a) for $x = 0.95$ (close to channel wall). (c) Same as (a) for $x = -0.95$ (close to channel wall).

Equation (4.17) is also shown in Fig. 3. The agreement of the asymptotic result (4.17) with the exact result (4.15) is seen to be very good.

The asymptotic formula (4.13) can be written in the following convenient form:

$$k'_R = k, \tag{4.18}$$

$$k'_I = \left(\frac{\delta'}{\delta}\right) F(k\delta), \tag{4.19}$$

where δ is the local filter width given by (2.10),

$$F(x) = x\left[\frac{\int_{-\infty}^{+\infty} \zeta G(\zeta)\sin(x\zeta)\,d\zeta}{\int_{-\infty}^{+\infty} G(\zeta)\cos(x\zeta)\,d\zeta}\right], \tag{4.20}$$

and the suffixes R and I denote real and imaginary parts respectively. Thus, to a very good approximation, the commutation error is seen to be purely dissipative in nature, in contrast to the central differencing error which is dispersive. The commutation error vanishes in regions where $\delta' = 0$ (such as at the center of a channel). From the example above it is clear that for the top-hat filter,

$$F(k\delta) = 1 - \frac{k\delta}{2}\cot\left(\frac{k\delta}{2}\right) = \frac{(k\delta)^2}{12} + \frac{(k\delta)^4}{720} + \cdots. \tag{4.21}$$

A simple calculation shows that, for the Gaussian filter (2.3),

$$F(k\delta) = \frac{(k\delta)^2}{4}. \tag{4.22}$$

5. HIGHER ORDER CORRECTIONS TO THE COMMUTATION ERROR

We have shown in the previous section that $\mathscr{C}[\psi] \approx \psi\mathscr{F}_0(k\Delta)$ and $\mathscr{F}_0(k\Delta) \sim (k\Delta)^2$ at leading order in $k\Delta$. In this section we shall attempt to approximate the commutation error $\mathscr{C}[\psi]$ by an expression involving $\overline{\psi}$ and its derivatives such that the residual is of order $(k\Delta)^4$. The procedure can be readily generalized to represent $\overline{\psi'(x)}$ in terms of $\overline{\psi}'(x)$ and higher derivatives of $\overline{\psi}(x)$ such that the error in the approximation is at most of order $(k\Delta)^{2m}$, where m is any positive integer.

We have, upon expanding the exponential in (4.6) and noting that $G(\zeta)$ is a symmetric function,

$$\mathscr{F}(x) = ix\int_{-\infty}^{+\infty} \zeta^2 G(\zeta)\,d\zeta - \frac{ix^3}{3!}\int_{-\infty}^{+\infty} \zeta^4 G(\zeta)\,d\zeta + \cdots. \tag{5.1}$$

Substitution of (5.1) in (4.5) gives

$$\mathscr{C}[\psi] = -(k\Delta)^2 \frac{f''}{(f')^3}\psi\int_{-\infty}^{+\infty} \zeta^2 G(\zeta)\,d\zeta + O(k\Delta)^4. \tag{5.2}$$

From (4.10),

$$\overline{\psi}(x) = \int_{-\infty}^{+\infty} G(\zeta)\psi\left(x + \frac{\Delta\zeta}{f'} + \cdots\right)d\zeta. \tag{5.3}$$

On substituting $\psi = \hat{\psi}_k \exp(ikx)$ in (5.3) and differentiating twice with respect to x we have

$$\overline{\psi}''(x) = -k^2\psi\left[1 - \alpha\frac{(k\Delta)^2}{2f'^2} + O(k\Delta)^4\right], \tag{5.4}$$

where

$$\alpha = \int_{-\infty}^{+\infty} \zeta^2 G(\zeta)\,d\zeta \tag{5.5}$$

and $\Delta \ll k\Delta$ has been assumed. Equation (5.4) implies that

$$-k^2\psi = \overline{\psi}''(x) + O(k\Delta)^2. \tag{5.6}$$

On substituting (5.6) in (5.2) we get

$$\mathscr{C}[\psi] = \alpha\frac{f''}{f'^3}\Delta^2\overline{\psi}''(x) + O(k\Delta)^4. \tag{5.7}$$

Thus,

$$\overline{\frac{d\psi}{dx}} = \frac{d\overline{\psi}}{dx} + \alpha\frac{f''}{f'^3}\Delta^2\frac{d^2\overline{\psi}}{dx^2} + O(k\Delta)^4. \tag{5.8}$$

The procedure can be continued to extend the accuracy of the representation to any order in $k\Delta$. Equation (5.8) can also be written in terms of the local grid spacing $\delta(x)$ as follows:

$$\overline{\frac{d\psi}{dx}} = \frac{d\overline{\psi}}{dx} - \alpha\delta^2\left(\frac{\delta'}{\delta}\right)\frac{d^2\overline{\psi}}{dx^2} + O(k\delta)^4. \tag{5.9}$$

Equation (5.9) was established only for the function (4.1). However, it is clearly valid for any linear superposition of functions of the type (4.1), that is, any function that admits a Fourier representation.

6. PHYSICAL INTERPRETATION OF THE HIGHER ORDER TERMS

It was shown in the last section that the application of the filtering operation to a differential equation generates higher spatial derivatives in the equation for the filtered field. What is the physical meaning of these higher order terms? In this section we address this issue with the help of a simple example.

Let us consider the one-dimensional wave equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \tag{6.1}$$

in the domain $(-\infty, +\infty)$, with the initial condition

$$u(x, 0) = u_0(x). \tag{6.2}$$

On applying the filtering operation (2.12) to Eq. (6.1) and on using (5.9) we have

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial \overline{u}}{\partial x} = \nu\frac{\partial^2 \overline{u}}{\partial x^2}, \tag{6.3}$$

where

$$\nu = \alpha\delta^2\left(\frac{\delta'}{\delta}\right). \tag{6.4}$$

The coefficient ν is small so that only the short wavelengths are significantly affected by the dissipation term on the right-hand side of (6.3). For the sake of definiteness, let us assume as an example the situation where the local filter width δ varies with position as

$$\delta = \delta_0\sqrt{1 + bx}, \tag{6.5}$$

where b and δ_0 are positive constants. Equation (6.5) clearly cannot be valid over the entire domain since the quantity under the square root becomes negative for large negative values of x. However, we will consider the initial waveform to be localized on the positive side of the x-axis and, since the wave described by (6.1) propagates from left to right, the values of $\delta(x)$ for large negative x will be irrelevant. (One can for example assume $\delta(x)$ to be given by (6.5) for large positive x and assume $\delta(x)$ to asymptotically approach δ_0 for large negative x without affecting the validity of the analysis that follows.) On substituting (6.5) in (6.4), we see that for this choice of $\delta(x)$, $\nu = \alpha b\delta_0^2/2$ is position independent. Therefore, Eq. (6.3) can be readily solved:

$$\bar{u}(x, t) = \int_{-\infty}^{+\infty} A_k e^{-\nu k^2 t} e^{ik(x-t)}\, dk \tag{6.6}$$

where

$$A_k = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \bar{u}_0(x) e^{-ikx}\, dx. \tag{6.7}$$

If the initial waveform is Gaussian,

$$\bar{u}_0(x) = \frac{1}{\sigma_0\sqrt{2\pi}}\exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right], \tag{6.8}$$

then a straightforward evaluation of the integrals in (6.6) and (6.7) gives

$$\bar{u}(x, t) = \frac{1}{\sigma_t\sqrt{2\pi}}\exp\left[-\frac{(x-x_0-t)^2}{2\sigma_t^2}\right] \tag{6.9}$$

where

$$\sigma_t = \sqrt{\sigma_0^2 + 2\nu t}. \tag{6.10}$$

Thus, even though u itself propagates from left to right unchanged in form, $\bar{u}$ slowly spreads as it propagates.

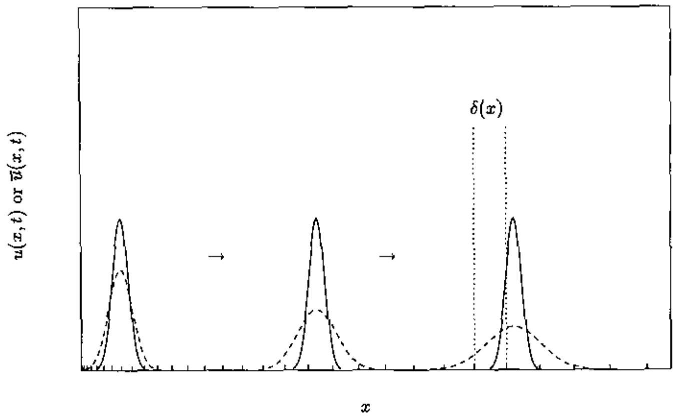

FIG. 4. A schematic diagram representing the spreading of a Gaussian wavepacket due to increasing filter width. The solid line is $u(x, t)$ and the dotted line is $\bar{u}(x, t)$.

The physical reason for this result is apparent from Fig. 4. The filtering operation "smears" the field $u(x, t)$ by an amount that increases with the filter width. As the pulse travels to the right, it encounters ever-increasing filter widths and consequently spreads with time. The validity of this interpretation can be checked by directly computing the "true field" $u(x, t)$ at time t and filtering it with the local filter function. We will consider G to be the Gaussian filter (2.3). Then to a first approximation, $\tilde{G}$ (see Section 2) is a Gaussian (see Eq. (2.16)) with standard deviation given by half the local filter width $\delta(x_0)/2 = (\delta_0\sqrt{1 + bx_0})/2$. Let us consider an initial field

$$u_0(x) = \frac{1}{\sigma_*\sqrt{2\pi}}\exp\left[-\frac{(x-x_0)^2}{2\sigma_*^2}\right]. \tag{6.11}$$

On recalling that the convolution of two Gaussians of means μ_1 and μ_2 and standard deviations σ_1 and σ_2 is again a Gaussian with mean $\mu_1 + \mu_2$ and standard deviation $\sqrt{\sigma_1^2 + \sigma_2^2}$, we deduce that $\bar{u}(x, 0)$ is a Gaussian with mean at $x = x_0$ and standard deviation

$$\sigma_0 = \sqrt{\sigma_*^2 + \frac{1}{4}\delta_0^2(1 + bx_0)}. \tag{6.12}$$

The solution of the wave equation (6.1) with (6.11) as initial condition is

$$u(x, t) = \frac{1}{\sigma_*\sqrt{2\pi}}\exp\left[-\frac{(x-x_0-t)^2}{2\sigma_*^2}\right]. \tag{6.13}$$

Once again, $\tilde{G}$ at $x = x_0 + t$ may be approximated by a Gaussian with standard deviation given by half the local filter width, which in this case is $\delta(x_0 + t)/2 = (\delta_0\sqrt{1 + bx_0 + bt})/2$. Therefore, $\bar{u}(x, t)$ is a Gaussian with mean at $x = x_0 + t$ and standard deviation

$$\sigma_t = \sqrt{\sigma_0^2 + \frac{1}{4}\delta_0^2(1 + bx_0) + \frac{1}{4}\delta_0^2 bt}. \quad (6.14)$$

On using (6.12) in (6.14) and noting that for the Gaussian filter $\alpha = \frac{1}{4}$ (α is the square of the standard deviation) so that $\nu = b\delta_0^2/8$, we deduce that

$$\sigma_t = \sqrt{\sigma_0^2 + 2\nu t}.$$

Thus, we recover precisely the same result that was obtained by directly solving Eq. (6.3) for the filtered field.

7. GENERALIZATION TO THREE SPACE DIMENSIONS

7.1. *Defining the Filter*

Let us consider curvilinear grids defined by the coordinate planes

$$H_1(x_1, x_2, x_3) = \text{constant}, \quad (7.1)$$

$$H_2(x_1, x_2, x_3) = \text{constant}, \quad (7.2)$$

$$H_3(x_1, x_2, x_3) = \text{constant}, \quad (7.3)$$

where x_1, x_2, and x_3 are rectilinear coordinates in physical space. Let us also introduce a new "computational space" $X_1X_2X_3$ through the mapping

$$X_1 = H_1(x_1, x_2, x_3), \quad (7.4)$$

$$X_2 = H_2(x_1, x_2, x_3), \quad (7.5)$$

$$X_3 = H_3(x_1, x_2, x_3), \quad (7.6)$$

which maps the physical space domain into $\mathbf{R}^3$ meshed with a uniform grid of spacing Δ. We will first define a filtering operation that is appropriate for use with this grid. Next we give a method of computing the commutation errors in terms of the resolved fields to any given order in accuracy.

Following the usual procedure (see Section 2), we first transform the field to be filtered, $\psi(\mathbf{x})$, from the physical to the "computational" space

$$\psi(\mathbf{x}) \to \psi(\mathbf{h}(\mathbf{X})),$$

where $\mathbf{h}$ is the inverse of $\mathbf{H}$. Next, we filter the field in computational space following the usual definition of filtering for a uniform grid,

$$\psi(\mathbf{h}(\mathbf{X})) \to \frac{1}{\Delta^3}\int \prod_{i=1}^{3} G\left(\frac{X_i - X_i'}{\Delta}\right) \psi(\mathbf{h}(\mathbf{X}'))\, d^3\mathbf{X}'.$$

Here G is the one-dimensional filter function as defined in Section 2. Finally, we transform back to physical space to get the filtered field,

$$\bar{\psi}(\mathbf{x}) = \frac{1}{\Delta^3}\int \prod_{i=1}^{3} G\left(\frac{H_i(\mathbf{x}) - X_i'}{\Delta}\right) \psi(\mathbf{h}(\mathbf{X}'))\, d^3\mathbf{X}'. \quad (7.7)$$

Equation (7.7) may also be written as

$$\bar{\psi}(\mathbf{x}) = \frac{1}{\Delta^3}\int \prod_{i=1}^{3} G\left(\frac{H_i(\mathbf{x}) - H_i(\mathbf{x}')}{\Delta}\right) \psi(\mathbf{x}')J(\mathbf{x}')\, d^3\mathbf{x}', \quad (7.8)$$

where $J(\mathbf{x})$ is the Jacobian of the transformation (7.4)–(7.6).

7.2. *The Commutation Error at Lowest Order*

Equation (7.7) gives, on differentiation,

$$\frac{\partial\bar{\psi}}{\partial x_k} = \frac{1}{\Delta^3}\int \frac{1}{\Delta} G'\left(\frac{H_j(\mathbf{x}) - X_j'}{\Delta}\right) \times \prod_{\substack{i=1\\ i\neq j}}^{3} G\left(\frac{H_i(\mathbf{x}) - X_i'}{\Delta}\right) H_{j,k}(\mathbf{x})\psi(\mathbf{h}(\mathbf{X}'))\, d^3\mathbf{X}'. \quad (7.9)$$

Throughout this paper we will be following tensor notation in which a comma followed by one or more indices denotes differentiation with respect to the corresponding variables. For example, $F_{i,j} \equiv \partial F_i/\partial x_j$. Unless otherwise stated, the summation convention is implied. From (7.9) we obtain, after using

$$\frac{1}{\Delta} G'\left(\frac{H_j(\mathbf{x}) - X_j'}{\Delta}\right) = -\frac{\partial}{\partial X_j'} G\left(\frac{H_j(\mathbf{x}) - X_j'}{\Delta}\right) \quad (7.10)$$

and integration by parts and noting that the boundary terms vanish (since any finite boundary is mapped to infinity by $\mathbf{H}$),

$$\begin{aligned}\frac{\partial\bar{\psi}}{\partial x_k} &= \frac{1}{\Delta^3}\int \prod_{i=1}^{3} G\left(\frac{H_i(\mathbf{x}) - X_i'}{\Delta}\right) H_{j,k}(\mathbf{x}) \frac{\partial}{\partial X_j'} \psi(\mathbf{h}(\mathbf{X}'))\, d^3\mathbf{X}' \\ &= \frac{1}{\Delta^3}\int \prod_{i=1}^{3} G\left(\frac{H_i(\mathbf{x}) - X_i'}{\Delta}\right) H_{j,k}(\mathbf{x}) h_{m,j}(\mathbf{X}')(\partial_m\psi)_{\mathbf{h}(\mathbf{X}')}\, d^3\mathbf{X}' \end{aligned} \quad (7.11)$$

where $(\partial_m\psi)_{\mathbf{h}(\mathbf{X}')}$ denotes the function $\partial_m\psi$ evaluated at $\mathbf{h}(\mathbf{X}')$. We define the commutation error as

$$C_k[\psi(\mathbf{x})] \equiv \left(\overline{\frac{\partial\psi}{\partial x_k}}\right) - \left(\frac{\partial\bar{\psi}}{\partial x_k}\right) \quad (7.12)$$

where $k = 1, 2$, or 3. Therefore, on using (7.7) and (7.11),

$$C_k[\psi(\mathbf{x})] = \frac{1}{\Delta^3}\int\prod_{i=1}^{3} G\left(\frac{H_i(\mathbf{x}) - X'_i}{\Delta}\right) \times (\partial_m\psi)_{\mathbf{h}(\mathbf{X}')}[\delta_{km} - H_{j,k}(\mathbf{h}(\mathbf{X}))h_{m,j}(\mathbf{X}')]\, d^3\mathbf{X}'. \tag{7.13}$$

If we introduce the new variable

$$\mathbf{Z} = \frac{\mathbf{X}' - \mathbf{X}}{\Delta}, \tag{7.14}$$

then (7.13) becomes

$$C_k[\psi(\mathbf{x})] = \int\prod_{i=1}^{3} G(\mathbf{Z})(\partial_m\psi)_{\mathbf{h}(\mathbf{X}+\Delta\mathbf{Z})}[\delta_{km} - H_{j,k}(\mathbf{h}(\mathbf{X}))h_{m,j}(\mathbf{X}+\Delta\mathbf{Z})]\, d^3\mathbf{Z}. \tag{7.15}$$

On using a Taylor series expansion in Δ we obtain

$$h_{m,j}(\mathbf{X}+\Delta\mathbf{Z}) = h_{m,j}(\mathbf{X}) + \Delta Z_l h_{m,jl}(\mathbf{X}) + \cdots. \tag{7.16}$$

Since $\mathbf{h}$ is the inverse of $\mathbf{H}$, it follows that

$$h_{m,j}(\mathbf{H}(\mathbf{x}))H_{j,k}(\mathbf{x}) = h_{m,j}(\mathbf{X})H_{j,k}(\mathbf{h}(\mathbf{X})) = \delta_{mk}. \tag{7.17}$$

Using (7.16) and (7.17) we derive

$$\begin{aligned} H_{j,k}(\mathbf{h}(\mathbf{X}))h_{m,j}(\mathbf{X}+\Delta\mathbf{Z}) &= h_{m,j}(\mathbf{X})H_{j,k}(\mathbf{h}(\mathbf{X})) \\ &\quad + \Delta Z_l h_{m,jl}(\mathbf{X})H_{j,k}(\mathbf{h}(\mathbf{X})) + \cdots \\ &= \delta_{km} + \Delta Z_l h_{m,jl}(\mathbf{X})H_{j,k}(\mathbf{h}(\mathbf{X})) + \cdots. \end{aligned} \tag{7.18}$$

Similarly,

$$(\partial_m\psi)_{\mathbf{h}(\mathbf{X}+\Delta\mathbf{Z})} = (\partial_m\psi)_{\mathbf{h}(\mathbf{X})} + \Delta Z_l h_{p,l}(\mathbf{X})(\partial_{mp}\psi)_{\mathbf{h}(\mathbf{X})} + \cdots. \tag{7.19}$$

On substituting (7.18) and (7.19) in (7.15) we obtain

$$C_k[\psi] = -\Delta h_{m,jl}(\mathbf{H}(\mathbf{x}))H_{j,k}(\mathbf{x})(\partial_m\psi)_{\mathbf{x}} \times \int\prod_{i=1}^{3} G(Z_i)Z_l\, d^3\mathbf{Z} + O(\Delta^2). \tag{7.20}$$

Now, by symmetry of the filter G,

$$\int\prod_{i=1}^{3} G(Z_i)Z_l\, d^3\mathbf{Z} = 0. \tag{7.21}$$

Therefore,

$$C_k[\psi] \sim O(\Delta^2). \tag{7.22}$$

7.3. *Higher Order Corrections*

Following the approach in Section 5, we consider the wave

$$\psi(\mathbf{x}) = \hat{\psi}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}). \tag{7.23}$$

On substituting (7.23) in (7.15), we obtain

$$C_k[\psi] = \int\prod_{i=1}^{3} G(Z_i)ik_m\hat{\psi}_k \exp(i\mathbf{k}\cdot\mathbf{h}(\mathbf{X}+\Delta\mathbf{Z})) \times [\delta_{km} - H_{j,k}(\mathbf{h}(\mathbf{X}))h_{m,j}(\mathbf{X}+\Delta\mathbf{Z})]\, d^3\mathbf{Z}. \tag{7.24}$$

On expanding $h_{m,j}(\mathbf{X}+\Delta\mathbf{Z})$ in a Taylor series in Δ, we obtain from (7.24)

$$C_k[\psi] = \mathcal{F}_0^{(k)}(\mathbf{k}\Delta) + \Delta\mathcal{F}_1^{(k)}(\mathbf{k}\Delta) + \cdots \tag{7.25}$$

where $\mathcal{F}_0^{(k)}(\mathbf{k}\Delta)$, $\mathcal{F}_1^{(k)}(\mathbf{k}\Delta)$, $\cdots$ are functions which contain Δ only in the combination $\mathbf{k}\Delta$. The first term is of particular interest to us and is expressed (on using (7.18)) as

$$\mathcal{F}_0^{(k)}(\mathbf{k}\Delta) = -ik_m\, \Delta h_{m,jq}(\mathbf{X})H_{j,k}(\mathbf{h}(\mathbf{X}))\psi(\mathbf{h}(\mathbf{X}))\mathcal{I}_q \tag{7.26}$$

where

$$\mathcal{I}_q \equiv \int\prod_{i=1}^{3} G(Z_i)Z_q \exp(i\,\Delta k_p h_{p,l}(\mathbf{X})Z_l)\, d^3\mathbf{Z}. \tag{7.27}$$

Since we have $\Delta \ll |\mathbf{k}|\Delta$ (see Section 5), we may drop every term in (7.25) except the first. Thus, $C_k[\psi] \approx \mathcal{F}_0^{(k)}(\mathbf{k}\Delta)$.

$C_k[\psi]$ can be obtained up to any order in $|\mathbf{k}|\Delta$ by expanding the exponential in (7.27) in powers of $|\mathbf{k}|\Delta$. Let us explicitly evaluate the lowest nonzero term by way of example. On expanding the exponential in (7.27) in a Taylor series,

$$\begin{aligned} \mathcal{I}_q &\approx i\,\Delta k_p h_{p,l}(\mathbf{X})\int\prod_{i=1}^{3} G(Z_i)Z_q Z_l\, d^3\mathbf{Z} \\ &= i\alpha\,\Delta k_p h_{p,q}(\mathbf{X}). \end{aligned} \tag{7.28}$$

Here α is given by (5.5) and we have used

$$\int\prod_{i=1}^{3} G(Z_i)Z_q Z_l\, d^3\mathbf{Z} = \alpha\delta_{ql}. \tag{7.29}$$

Thus,

$$C_k[\psi] = \alpha\Delta^2 k_m k_p h_{m,jq}(\mathbf{X}) h_{p,q}(\mathbf{X}) H_{j,k}(\mathbf{h}(\mathbf{X}))\psi(\mathbf{h}(\mathbf{X})) + O(|\mathbf{k}|\Delta)^4. \tag{7.30}$$

The last and final step is to express $k_m k_p \psi(\mathbf{h}(\mathbf{X}))$ in terms of some derivatives of $\overline{\psi}$. In order to do this we note that Eq. (7.7) may be written as

$$\begin{aligned}\overline{\psi}(\mathbf{x}) &= \int \prod_{i=1}^{3} G(Z_i)\psi(\mathbf{h}(\mathbf{X} + \Delta\mathbf{Z}))\, d^3\mathbf{Z} \\ &= \int \prod_{i=1}^{3} G(Z_i)\psi(\mathbf{h}(\mathbf{X}))\exp(ik_m\, \Delta h_{m,p}(\mathbf{X})Z_p)\, d^3\mathbf{Z} \\ &\quad + \Delta f_1(\mathbf{k}\Delta) + \cdots,\end{aligned} \tag{7.31}$$

where $f_1(\mathbf{k}\Delta)$ is some function containing Δ only in the combination $\mathbf{k}\Delta$ and likewise for the remaining terms. Thus,

$$\overline{\psi}(\mathbf{x}) \approx \psi(\mathbf{x}) J(\mathbf{k}\Delta) \tag{7.32}$$

where

$$J(\mathbf{k}\Delta) = \int \prod_{i=1}^{3} G(Z_i)\exp(i\,\Delta k_m\, h_{m,p}(\mathbf{X})Z_p)\, d^3\mathbf{Z}. \tag{7.33}$$

On noting that $J(\mathbf{k}\Delta) = 1 + O(|\mathbf{k}|\Delta)^2$ and $\psi_{,mp} = -k_m k_p \psi$, we have, from (7.32), $\overline{\psi}_{,mp} = -k_m k_p \overline{\psi} + O(|\mathbf{k}|\Delta)^2$. If we substitute this in (7.30), we obtain

$$C_k[\psi] = -\alpha\Delta^2 \Gamma_{kmp} \frac{\partial^2 \overline{\psi}}{\partial x_m \partial x_p} + O(|\mathbf{k}|\Delta)^4, \tag{7.34}$$

where

$$\Gamma_{kmp} = h_{m,jq}(\mathbf{H}(\mathbf{x})) h_{p,q}(\mathbf{H}(\mathbf{x})) H_{j,k}(\mathbf{x}). \tag{7.35}$$

Using (7.26) together with (7.32), an expression for $C_k[\psi]$ in terms of $\overline{\psi}$ can be written down to any order in Δ. Thus,

$$\overline{\partial_k \psi} = (\partial_k - \alpha\, \Delta^2 \Gamma_{kmn} \partial^2_{mn} + \cdots)\overline{\psi}. \tag{7.36}$$

8. THE QUESTION OF BOUNDARY CONDITIONS

We have shown that the effect of a nonuniform filter is accounted for in the equation for the filtered field through the introduction of higher order spatial derivatives. This implies that additional boundary conditions are required to uniquely determine the solution. In this section we show how such additional boundary conditions can be obtained. The implementation of even the "usual" boundary conditions in the Navier–Stokes equations often involves subtle numerical difficulties (see e.g. [4]). Therefore, the necessity of having to take into account these additional boundary conditions might be quite undesirable from the point of view of practical computations. It is shown that if the modified equations are solved perturbatively by asymptotic expansion with respect to the small parameter Δ^2, the equations that need to be solved at any given step in the procedure are of the same order in spatial derivatives as the original system. Thus, the perturbative solution does not require the specification of additional boundary conditions. The extra boundary conditions required for the full solution are automatically satisfied when a certain form is assumed for the perturbative solution. The issues are clearly understood in the context of a simple example problem.

Let us consider the equation

$$\frac{du}{dx} = 0 \tag{8.1}$$

in $[0, +\infty)$ with the boundary condition

$$u(0) = 1. \tag{8.2}$$

The exact solution is clearly $u(x) = 1$, which implies $\overline{u}(x) = 1$. On applying the filtering operation (2.12) and using (5.8) we have

$$\alpha \frac{f''}{f'^3} \Delta^2 \frac{d^2\overline{u}}{dx^2} + \frac{d\overline{u}}{dx} = 0. \tag{8.3}$$

Since $u \to \overline{u}$ at the wall, (8.2) implies

$$\overline{u}(0) = 1. \tag{8.4}$$

By definition, f must be singular at the origin. If the singularity is logarithmic, then $f''/f'^3 \sim -x$. However, if $f \sim -x^{-p}$ ($p > 0$) then $f''/f'^3 \sim -x^{2p+1}$. In either case, $f''/f'^3 \to 0$ at the boundary (as it must, since the filtering kernel $\tilde{G}(x, y) \to \delta(x - y)$ at the boundary, so that the filtered and unfiltered fields become identical in this limit and hence the extra terms must drop out). Therefore, if we require that $\overline{u}$ together with its derivatives should remain finite at the boundary, then we have from (8.3) that

$$\overline{u}'(0) = 0. \tag{8.5}$$

Equation (8.5) is the required additional boundary condition. The solution of (8.3) subject to the boundary conditions (8.4) and (8.5) is clearly $\overline{u}(x) = 1$. Thus, the exact solution is recovered.

The solution can also be obtained by treating the term with coefficient Δ^2 as a small perturbation. Thus, on substituting

$$\overline{u} = \overline{u}_0(x) + \Delta^2\overline{u}_1(x) + \Delta^4\overline{u}_2(x) + \cdots \tag{8.6}$$

in (8.3) and (8.4), one obtains at lowest order

$$\frac{d\overline{u}_0}{dx} = 0 \tag{8.7}$$

and

$$\overline{u}_0(0) = 1. \tag{8.8}$$

Therefore,

$$\overline{u}_0(x) = 1. \tag{8.9}$$

At the next order, we have from (8.3) and (8.4)

$$\frac{d\overline{u}_1}{dx} = -\alpha\frac{f''}{f'^3}\frac{d^2\overline{u}_0}{dx^2} \tag{8.10}$$

and

$$\overline{u}_1(0) = 0. \tag{8.11}$$

Equations (8.9), (8.10) and (8.11) imply

$$\overline{u}_1(x) = 0. \tag{8.12}$$

It is not meaningful to consider any higher order terms since (8.3) itself is only accurate to order Δ^2. Therefore, the solution obtained by the perturbation method is

$$\overline{u}(x) = 1 + O(\Delta^4). \tag{8.13}$$

If all the higher order terms were included in (8.3), the perturbation method would give $\overline{u}_0(x) = 1$ and $\overline{u}_n(x) = 0$ for all $n \geq 1$. Hence, the exact solution is recovered. It is important to note that, in the perturbative method, one solves a first order equation at any given step in the process, so that additional boundary conditions are not required. However, (8.5) is automatically satisfied by the perturbative solution. The reason is that (8.5) follows from (8.3) on assuming that the second derivative of $\overline{u}$ is finite at the boundary and this condition has been implicitly assumed in writing (8.10).

9. LES OF INHOMOGENEOUS TURBULENT FLOWS—THE BASIC EQUATIONS

Incompressible Navier–Stokes turbulence is described by the basic equations

$$\partial_t u_i + \partial_j(u_i u_j) = -\partial_i p + Re^{-1}\partial_{kk}u_i \tag{9.1}$$

and

$$\partial_i u_i = 0. \tag{9.2}$$

On taking the divergence of (9.1) and using (9.2) we obtain

$$\nabla^2 p = -\partial^2_{ij}(u_i u_j). \tag{9.3}$$

In numerical computations (9.1) is usually solved in conjunction with (9.3) and thereby (9.2) is automatically satisfied, provided the initial velocity field is divergence free. We will now derive the corresponding equations that are satisfied by the filtered fields $\overline{u}_i$ and $\overline{p}$. In order to do this, we apply the filtering operation (7.8) on both sides of Eqs. (9.1) and (9.2) and make use of (7.36) to take the filtering operation inside the spatial differentiation operator.

It is however convenient to first introduce the operators $\mathcal{D}_i$ (where $i = 1, 2, 3$) such that

$$\overline{\partial_i\psi} = \mathcal{D}_i\overline{\psi}. \tag{9.4}$$

From (7.36), $\mathcal{D}_i$ has the expansion

$$\mathcal{D}_i = \partial_i - \alpha\Delta^2\Gamma_{ijk}\partial^2_{jk} + \cdots. \tag{9.5}$$

It follows from (9.4) that the operators $\mathcal{D}_i$ must commute with each other; that is,

$$[\mathcal{D}_i, \mathcal{D}_j] \equiv \mathcal{D}_i\mathcal{D}_j - \mathcal{D}_j\mathcal{D}_i = 0. \tag{9.6}$$

To see that this must be true, we simply use (9.4) on both sides of the identity

$$\overline{\frac{\partial^2\psi}{\partial x_i \partial x_j}} = \overline{\frac{\partial^2\psi}{\partial x_j \partial x_i}}. \tag{9.7}$$

Then the left-hand side becomes $\mathcal{D}_i\mathcal{D}_j\overline{\psi}$, the right-hand side becomes $\mathcal{D}_j\mathcal{D}_i\overline{\psi}$, and hence (9.6) must be true. In order for the expansion (9.5) to be consistent with (9.6), we must have

$$[\mathcal{D}_i^*, \mathcal{D}_j^*] \sim \Delta^4, \tag{9.8}$$

where

$$\mathcal{D}_i^* \equiv 1 - \alpha\Delta^2\Gamma_{ijk}\partial^2_{jk}. \tag{9.9}$$

Indeed, from (9.5) and (9.6),

$$[\mathcal{D}_i, \mathcal{D}_j] = [\mathcal{D}_i^*, \mathcal{D}_j^*] + O(\Delta^4) = 0, \tag{9.10}$$

and hence (9.8) must be true. It can be directly verified that the expression for Γ_{ijk} given by (7.35) is indeed consistent with (9.10), and the proof of this is presented in the Appendix.

On applying the filtering operation ($\psi \rightarrow \overline{\psi}$) to both sides of (9.1) and introducing the sgs stress tensor

$$\tau_{ij} \equiv \overline{u_i u_j} - \overline{u}_i \overline{u}_j, \tag{9.11}$$

we have

$$\partial_t \overline{u}_i + \mathfrak{D}_j(\overline{u}_i \overline{u}_j) = -\mathfrak{D}_i \overline{p} - \mathfrak{D}_j \tau_{ij} + Re^{-1} \mathfrak{D}_k \mathfrak{D}_k \overline{u}_i. \tag{9.12}$$

Note that in deriving (9.12) use has been made of the fact that the operators $\mathfrak{D}_i$ commute with each other. Similarly, on applying the filtering operation to (9.2), we derive

$$\mathfrak{D}_i \overline{u}_i = 0. \tag{9.13}$$

The equation for the filtered pressure can be derived either by applying the operator $\mathfrak{D}_i$ to (9.12) and using (9.13) or by applying the filtering operation directly to (9.3). It is readily verified that both methods give the same equation

$$\mathfrak{D}_k \mathfrak{D}_k \overline{p} = -\mathfrak{D}_i \mathfrak{D}_j (\overline{u}_i \overline{u}_j + \tau_{ij}) \tag{9.14}$$

for computing the pressure. If some sgs model $\tau_{ij} = \tau_{ij}[\mathbf{u}]$ is used in (9.12)–(9.14) and suitable boundary conditions are assumed, the LES fields $\overline{p}$ and $\overline{u}_i$ can be uniquely determined.

Equations (9.12) and (9.13) are higher order in spatial derivatives than the incompressible Navier–Stokes equations and therefore require the specification of additional boundary conditions. These can be derived in the manner explained in Section 8. Thus, if only corrections to order Δ^2 are retained, the additional boundary conditions are

$$\partial_t \overline{u}_i + \partial_j (\overline{u}_i \overline{u}_j) = -\partial_i \overline{p} - \partial_j \tau_{ij} + Re^{-1} \partial^2_{kk} \overline{u}_i \tag{9.15}$$

and

$$\partial_i \overline{u}_i = 0 \tag{9.16}$$

at the boundary.

The necessity of specifying additional boundary conditions can be avoided (see Section 8) if (9.12)–(9.13) are solved perturbatively by treating Δ^2 as a small parameter. As an example, suppose that we must solve the LES equations in some domain with the condition that the velocities must vanish on some surface $\mathcal{S}$. Then, we have

$$u_i(\mathbf{x} = \mathcal{S}) = 0 = \overline{u}_i(\mathbf{x} = \mathcal{S}). \tag{9.17}$$

On expanding $\overline{u}_i$ and $\overline{p}$ in asymptotic series

$$\overline{p} = \overline{p}^{(0)} + \Delta^2 \overline{p}^{(1)} + \cdots \tag{9.18}$$

$$\overline{u}_i = \overline{u}_i^{(0)} + \Delta^2 \overline{u}_i^{(1)} + \cdots, \tag{9.19}$$

and on substituting (9.18) and (9.19) in (9.12), (9.13), and (9.17), we have at the lowest order

$$\partial_t \overline{u}_i^{(0)} + \partial_j (\overline{u}_i^{(0)} \overline{u}_j^{(0)}) = -\partial_i \overline{p}^{(0)} - \partial_j \tau_{ij}^{(0)} + Re^{-1} \partial^2_{kk} \overline{u}_i^{(0)}, \tag{9.20}$$

$$\partial_i \overline{u}_i^{(0)} = 0, \tag{9.21}$$

and

$$\overline{u}_i^{(0)}(\mathbf{x} = \mathcal{S}) = 0. \tag{9.22}$$

Here $\tau_{ij}^{(0)}, \tau_{ij}^{(1)}, \cdots$ are the expansion coefficients obtained on substituting (9.19) into the sgs model $\tau_{ij}[\mathbf{u}]$. At the next order in Δ^2 (9.12) gives

$$\begin{aligned} &\partial_t \overline{u}_i^{(1)} + \partial_j (\overline{u}_i^{(0)} \overline{u}_j^{(1)}) + \partial_j (\overline{u}_i^{(1)} \overline{u}_j^{(0)}) + \partial_i \overline{p}^{(1)} \\ &\quad + \partial_j \tau_{ij}^{(1)} - Re^{-1} \partial_{kk} \overline{u}_i^{(1)} = \alpha f_i, \end{aligned} \tag{9.23}$$

where

$$\begin{aligned} f_i = {} & \Gamma_{jmn} \partial^2_{mn} (\overline{u}_i^{(0)} \overline{u}_j^{(0)}) + \Gamma_{imn} \partial^2_{mn} \overline{p}^{(0)} + \Gamma_{jmn} \partial^2_{mn} \tau_{ij}^{(0)} \\ & - Re^{-1} \Gamma_{kmn,k} \partial^2_{mn} \overline{u}_i^{(0)} - 2 Re^{-1} \Gamma_{kmn} \partial^3_{kmn} \overline{u}_i^{(0)} \end{aligned} \tag{9.24}$$

is a "forcing term" that is known from the solution at the previous order. Similarly, Eq. (9.13) gives

$$\partial_i \overline{u}_i^{(1)} = 0 \tag{9.25}$$

and Eq. (9.17) implies that

$$\overline{u}_i^{(1)}(\mathbf{x} = \mathcal{S}) = 0. \tag{9.26}$$

It should be noted that any basic Navier–Stokes numerical code can be used to solve (9.20)–(9.26) with no modification to its basic structure. The evaluation of the pressure and velocity fields are done twice instead of once every time step. First (9.20)–(9.22) are solved and the zeroth order fields are stored. Next, this information is used to solve (9.23)–(9.26) to determine the leading order correction.

The increase in numerical effort will be mainly determined by the number of nonzero components in the tensor Γ_{ijk}, which is a meausre of the complexity of the shape of the flow domain. In the direct method, a single evaluation is sufficient but the additional boundary conditions (9.15)–(9.16) must be explicitly enforced.

10. CONCLUSIONS

The method of large-eddy simulation is supposed to compute a filtered version of the true velocity field in a turbulent flow. In a flow with boundaries, the filter width must vary with position to reflect the changing length scales of the characteristic structures in the flow. A variable filter width invalidates the standard derivation of the large-eddy equations which were originally written down for a situation where the filter width is constant.

In this paper, the LES equations were derived for a variable filter width appropriate for general complex geometry flows. The main difficulty that arises in such a derivation is due to the fact that the operations of differentiation and filtering do not commute. In order to address this difficulty a new definition of the filtering operation which we call a second-order commuting filter (SOCF) was introduced. Using this definition it was shown that the commutation error is of order Δ^2 where Δ is the nondimensional grid spacing (that is, the ratio of the grid spacing in physical units and a characteristic length of the flow domain).

The above theory is applied to the Navier–Stokes equations and it is shown that the use of the standard large-eddy equations introduces an error that is no more than the error introduced by a second-order finite difference scheme used to discretize the LES equations. Such an error, however, might not be acceptable if one is using a higher order differencing scheme or a pseudo-spectral method. An asymptotic expansion for the commutation error was developed so that the commutation error can be approximated to any degree of accuracy in terms of the filtered fields. Thus, any number of higher order corrections can be added to the standard LES equations to ensure that the commutation error does not exceed the discretization error in a numerical simulation. The inclusion of such higher derivatives increases the spatial order of the differential equations so that additional boundary conditions are needed to obtain a unique solution. The required additional boundary conditions can be derived from the requirement that the filtered and unfiltered fields must become identical infinitesimally close to the boundary. Alternatively, one may take advantage of the smallness of the parameter Δ^2 and obtain a perturbative solution. In this method additional boundary conditions need not be enforced since at any given order in the perturbation series the differential equations to be solved have the same spatial order as the Navier–Stokes equations.

APPENDIX

It is shown in the text that in order for the asymptotic expansion (7.36) to be consistent with (9.6), we must have $[\mathfrak{D}_j^*, \mathfrak{D}_k^*] \sim \Delta^4$. Here we explicitly show that this consistency requirement is indeed satisfied.

On using the definition (9.9) we see that

$$\begin{aligned}\mathfrak{D}_j^*\mathfrak{D}_k^*\psi &= \partial^2_{jk}\psi - \alpha\Delta^2\partial_j(\Gamma_{kpq}\,\partial^2_{pq}\psi) \\ &\quad - \alpha\Delta^2\Gamma_{jmn}\,\partial^3_{mnk}\psi + O(\Delta^4) \qquad \text{(A.1)} \\ &= \partial^2_{jk}\psi - \alpha\Delta^2\Gamma_{kpq,j}\,\partial^2_{pq}\psi - \alpha\Delta^2\Gamma_{kpq}\,\partial^3_{pqj}\psi \\ &\quad - \alpha\Delta^2\Gamma_{jmn}\,\partial^3_{mnk}\psi + O(\Delta^4).\end{aligned}$$

On interchanging the indices j and k the first term on the right-hand side of (A.1) remains unchanged, whereas the third and fourth terms transform into each other. Therefore, we have

$$[\mathfrak{D}_j^*, \mathfrak{D}_k^*] = -\alpha\Delta^2(\Gamma_{kpq,j} - \Gamma_{jpq,k})\,\partial^2_{pq} + O(\Delta^4). \qquad \text{(A.2)}$$

We will now show that $\Gamma_{kpq,j} - \Gamma_{jpq,k}$ is antisymmetric with respect to the indices p and q. This will complete the proof since ∂^2_{pq} in (A.2) is symmetric with respect to p and q and hence the first term on the right-hand side of (A.2) will vanish on summing over p and q.

We obtain, upon differentiating (7.35) and using the chain rule,

$$\begin{aligned}\Gamma_{ijk,l} &= h_{j,mn\mu}H_{\mu,l}h_{k,n}H_{m,i} + h_{j,mn}h_{k,n\mu}H_{\mu,l}H_{m,i} \qquad \text{(A.3)} \\ &\quad + h_{j,mn}h_{k,n}H_{m,il},\end{aligned}$$

where it is understood that all H's are evaluated at $\mathbf{x}$ while all h's are evaluated at $H(\mathbf{x})$. On exchanging the indices i and l, the first term on the right of (A.3) becomes $h_{j,mn\mu}H_{\mu,i}h_{k,n}H_{m,l} = h_{j,\mu nm}H_{m,i}h_{k,n}H_{\mu,l} = h_{j,mn\mu}H_{\mu,l}h_{k,n}H_{m,i}$ which is the original expression. Thus, the first term is symmetric with respect to the indices i and l. The last term is obviously symmetric with respect to i and l. Therefore, the second term on the right of (A.3) is the only term that contributes to $\Gamma_{ijk,l} - \Gamma_{ljk,i}$, and we have

$$\Gamma_{ijk,l} - \Gamma_{ljk,i} = (h_{j,mn}h_{k,n\mu} - h_{j,\mu n}h_{k,nm})H_{\mu,l}H_{m,i}. \qquad \text{(A.4)}$$

The antisymmetry of $\Gamma_{ijk,l} - \Gamma_{ljk,i}$ with respect to j and k is now obvious since the first and the second term inside the parentheses in Eq. (A.4) transform into each other on exchanging j and k. This completes the proof.

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REFERENCES

1. A. A. Aldama, *Filtering Techniques for Turbulent Flow Simulation* (Lecture Notes in Engineering, Vol. 56, Springer-Verlag, New York/Berlin, 1990).
2. A. Leonard, *Adv. Geophys. A* **18,** 237 (1974).
3. P. Moin and J. Kim, *J. Fluid Mech.* **118,** 341 (1982).
4. P. Moin and J. Kim, *J. Comput. Phys.* **35,** 381 (1980).
5. P. Moin, W. C. Reynolds, and J. H. Ferziger, 1978 Large eddy simulation of incompressible turbulent channel flow, Dept. of Mech. Eng. Rep. TF12, Stanford University.