Multi-scale gradient expansion of the turbulent stress tensor

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Turbulent stress is the fundamental quantity in the filtered equation for large-scale velocity that reflects its interactions with small-scale velocity modes. We develop an expansion of the turbulent stress tensor into a double series of contributions from different scales of motion and different orders of space derivatives of velocity, a multi-scale gradient (MSG) expansion. We compare our method with a somewhat similar expansion that is based instead on defiltering. Our MSG expansion is proved to converge to the exact stress, as a consequence of the locality of cascade both in scale and in space. Simple estimates show, however, that the convergence rate may be slow for the expansion in spatial gradients of very small scales. Therefore, we develop an approximate expansion, based upon an assumption that similar or 'coherent' contributions to turbulent stress are obtained from disjoint subgrid regions. This coherent-subregions approximation (CSA) yields an MSG expansion that can be proved to converge rapidly at all scales and is hopefully still reasonably accurate. As an important first application of our methods, we consider the cascades of energy and helicity in three-dimensional turbulence. To first order in velocity gradients, the stress has three contributions: a tensile stress along principal directions of strain, a contractile stress along vortex lines, and a shear stress proportional to 'skew-strain'. While vortex stretching plays the major role in energy cascade, there is a second, less scale-local contribution from 'skew-strain'. For helicity cascade the situation is reversed, and it arises scale-locally from 'skew-strain' while the stress along vortex lines gives a secondary, less scale-local contribution. These conclusions are illustrated with simple exact solutions of three-dimensional Euler equations. In the first, energy cascade occurs by Taylor's mechanism of stretching and spin-up of small-scale vortices owing to large-scale strain. In the second, helicity cascade occurs by 'twisting' of small-scale vortex filaments owing to a large-scale screw.

1. Introduction

It is recognized that turbulent cascades are essentially multi-scale phenomena, and involve the coupling of modes at distinct scales. The property of *locality* implies that these interactions are mainly between adjacent scales (Eyink 2005). Of course, this locality is rather weak and modes at scales differing by an order of magnitude from a fixed scale can make a substantial contribution to transfer across that scale. In the filtering approach (Germano 1992), the nonlinear interaction between scales is embodied in the *turbulent stress tensor* $\boldsymbol{\tau}$ that appears in the equation for the velocity $\overline{\boldsymbol{u}}$, low-pass filtered at length scale ℓ. This stress is the contribution to spatial transport of large-scale momentum generated by quadratic self-coupling of the subfilter scales.

Because of the locality property, the subfilter modes that contribute most to the stress are those at scales only somewhat smaller than ℓ. This raises the hope that a *constitutive relation* may be constructed for the stress, if the adjacent small scales can be somehow estimated from the resolved modes. Unfortunately, it is not hard to see that eliminating the small scales produces a stress whose dependence upon the large-scale velocity $\bar{u}$ is, in general, spatially non-local, history-dependent and stochastic (Lindenberg, West & Kottalam 1987; Eyink 1996). Thus, an exact constitutive relation for the turbulent stress is formally available, but it is quite unwieldy and not of direct practical use.

In apparent contradiction to these remarks, several authors have developed a closed constitutive formula for the turbulent stress (Yeo & Bedford 1988; Leonard 1997; Carati, Winckelmans & Jeanmart 2001). The basic idea of their approach is to *defilter* $\bar{u}$ to obtain the unfiltered velocity field u and then to use the latter to calculate the stress. For many common filter kernels, it is possible to evaluate the resulting formula as a concrete expansion in powers of the filtered velocity gradients. Although nothing is proved about the convergence of this series, it seems, in principle, to provide a solution to the 'closure problem' of turbulence. However, as we argue at length below, this solution is illusory for several reasons. Most obviously, defiltering is not defined for all filter kernels. Furthermore, the defiltering operator, even when defined, is unbounded on the natural function spaces for the velocity field (e.g. finite-energy functions). Thus, the convergence cannot hold in general.

Nevertheless, it is an extremely attractive idea to develop an expansion for the stress in powers of the filtered velocity gradients. Similar expansions have proved useful in many areas of physics, e.g. for one-particle distribution functions in the solution of the Boltzmann equation (Enskog 1917; Chapman & Cowling 1939) or for Ginzburg–Landau free energies of superconductors (Gorkov 1959; Tewordt 1965). We shall here develop a convergent gradient expansion for the turbulent stress. It is somewhat more intricate than the expansion developed in Yeo & Bedford (1988), Leonard (1997) and Carati *et al.* (2001), since it is expressed by a summation simultaneously over the order of space gradients and over an integer index indicating the scale of motion involved. Thus, it is a *multi-scale gradient expansion*. This series expansion will be proved below to converge, as a consequence of the locality of the turbulent cascade both in space and in scale. Of course, the rate of convergence may be slow, especially for the Taylor expansion in space of small scales, so that very high-order gradients could be required to obtain an accurate result. We diagnose the reasons for potentially poor convergence, and, on that basis, develop also an approximate expansion which will converge rapidly at all scales. This approximation may give reasonable accuracy with just a few low-order gradients.

Because it is multi-scale, the expansion considered here does not by itself give a closed 'constitutive' relation for the stress. However, it may be a useful point of departure in developing a closure for the stress, if supplemented with a scheme to estimate subfilter velocity gradients in terms of filtered velocity gradients. This is in line with some large-eddy simulation (LES) approaches which construct subgrid-stress models by creating 'surrogate' subgrid modes. See Domaradzki & Saiki (1997), Misra & Pullin (1997), Scotti & Meneveau (1999), Burton *et al.* (2002), and, for an extensive review, Domaradzki & Adams (2002). Our emphasis in this paper is on fundamental physics rather than on closure models, but we hope to pursue this in future work. Even without a closure prescription, the formula we develop for the stress makes many testable predictions. Concrete conclusions will be deduced here for the joint cascade of energy and helicity in three space dimensions and, in a following

paper Eyink (2006), for the inverse energy cascade predicted in two dimensions by Kraichnan (1967).

The contents of this paper are as follows. In §2, we briefly review the filtering approach to turbulence. In §3, we develop our multi-scale gradient (MSG) expansion for the turbulent stress. In §4, we develop a more rapidly convergent but less systematic approximation, which we call the coherent-subregions approximate multi-scale gradient (CSA-MSG) expansion. In §5, we present the application of our method to three-dimensional energy and helicity cascades. Technical proofs and calculations are given in four Appendices.

2. Filtering approach and turbulent stress

We first give a general discussion of the mechanics of energy transfer between scales in a turbulent flow. Following Germano (1992), we resolve turbulent fields simultaneously in space and in scale using a simple filtering approach. We consider initially an arbitrary dimension d of space. Thus, we define a low-pass filtered velocity

$$\overline{\boldsymbol{u}}(\boldsymbol{x}) = \int \mathrm{d}^d\boldsymbol{r} \ G_\ell(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{x}+\boldsymbol{r}), \tag{2.1}$$

where G is a smooth mollifier or filtering function, non-negative, spatially well-localized, with unit integral $\int \mathrm{d}^d\boldsymbol{r} \ G(\boldsymbol{r})=1$. The function G_ℓ is rescaled with ℓ, as $G_\ell(\boldsymbol{r})=\ell^{-d}G(\boldsymbol{r}/\ell)$. Likewise, we can define a complementary high-pass filter by

$$\boldsymbol{u}'(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{x}) - \overline{\boldsymbol{u}}(\boldsymbol{x}). \tag{2.2}$$

If the above filtering operation is applied to the incompressible Navier–Stokes equation

$$\partial_t\boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla p + \nu\Delta\boldsymbol{u}, \tag{2.3}$$

with $\nabla\cdot\boldsymbol{u}=0$ determining the pressure p, then we obtain

$$\partial_t\overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}}\cdot\nabla)\overline{\boldsymbol{u}} = -\nabla\cdot\boldsymbol{\tau} - \nabla\overline{p} + \nu\Delta\overline{\boldsymbol{u}}, \tag{2.4}$$

where

$$\boldsymbol{\tau} = \overline{\boldsymbol{u}\boldsymbol{u}} - \overline{\boldsymbol{u}}\,\overline{\boldsymbol{u}} \tag{2.5}$$

is the *stress tensor* from the scales $<\ell$ removed by the filtering.

The equation for energy balance in the large scales is (Piomelli *et al.* 1991; Eyink 1995):

$$\partial_t e + \nabla\cdot\boldsymbol{J} = -\Pi - \nu|\nabla\overline{\boldsymbol{u}}|^2, \tag{2.6}$$

with large-scale *energy density* $e=(1/2)\overline{\boldsymbol{u}}^2$, spatial *energy transport* vector in the large scales $\boldsymbol{J} = (e+\overline{p})\overline{\boldsymbol{u}} + \overline{\boldsymbol{u}}\cdot\boldsymbol{\tau} - \nu\nabla e$, and scale-to-scale *energy flux*

$$\Pi = -\nabla\overline{\boldsymbol{u}} : \boldsymbol{\tau}. \tag{2.7}$$

The latter quantity is the rate of work done by the large-scale velocity gradient against the small-scale stress. Of course, it may be rewritten in various equivalent forms as

$$\Pi = -\nabla\overline{\boldsymbol{u}} : \overset{\circ}{\boldsymbol{\tau}} = -\overline{\boldsymbol{S}} : \boldsymbol{\tau} = -\overline{\boldsymbol{S}} : \overset{\circ}{\boldsymbol{\tau}}. \tag{2.8}$$

The first follows from incompressibility of the velocity field, where

$$\overset{\circ}{\boldsymbol{\tau}} = \boldsymbol{\tau} - (\mathrm{Tr}\,\boldsymbol{\tau})\boldsymbol{I}/d \tag{2.9}$$

is the so-called *deviatoric stress* (with $\boldsymbol{I}$ the $d \times d$ identity matrix). The second follows from symmetry of the stress tensor, where

$$\overline{S}_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \tag{2.10}$$

is the large-scale strain rate. The third follows from both properties combined.

The formula

$$\boldsymbol{\tau} = \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}) - \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}) \cdot \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}) \tag{2.11}$$

represents the stress as a tensor product of velocity increments $\delta \boldsymbol{u}(\boldsymbol{r}; \boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{x}+\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{x})$ averaged over the separation vector $\boldsymbol{r}$ with respect to filter function $G_\ell(\boldsymbol{r})$ at length-scale ℓ. It is easily verified by multiplying out the increments and integrating (Constantin, E & Titi 1994; Eyink 1995). This expression implies, as a direct consequence, the matrix positivity of the stress (Vreman, Geurts & Kuerten 1994). It was also the crucial point of departure in our discussion of scale locality properties in Eyink (2005). This same formula plays a central role in our development of the multi-scale gradient expansion in this work. A decomposition of (2.11) that we find useful is

$$\boldsymbol{\tau} = \boldsymbol{\varrho} - \boldsymbol{u}' \boldsymbol{u}', \tag{2.12}$$

where

$$\boldsymbol{\varrho}(\boldsymbol{x}) = \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}; \boldsymbol{x}) \delta \boldsymbol{u}(\boldsymbol{r}; \boldsymbol{x}), \tag{2.13}$$

and

$$\boldsymbol{u}'(\boldsymbol{x}) = - \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}(\boldsymbol{r}; \boldsymbol{x}). \tag{2.14}$$

It is easy to check that $\boldsymbol{u}'(\boldsymbol{x})$ in (2.14) coincides with the high-pass filtered field in (2.2), so that $-\boldsymbol{u}' \boldsymbol{u}'$ represents a 'fluctuation' contribution to the subscale stress, while $\boldsymbol{\varrho}$ represents a 'systematic' contribution from the spatially averaged positive-definite tensor product of velocity increments.

3. Convergent expansion in scale and space

In this section, we develop our convergent expansion for the turbulent stress. The key to this convergence is the locality of the stress both in scale and in space. Therefore, we discuss in turn these two properties, develop from them the resulting expansions, and establish their convergence properties.

3.1. *Locality in scale*

Scale-locality is the property that only modes from length scales near the filter scale ℓ contribute predominantly to the stress. We have given a rigorous proof of this property, assuming only the inertial-range scaling laws that are observed in experiment and simulations (Eyink 2005) and we refer to that work for a more complete discussion. Here, we merely recall that locality properties were demonstrated there by introducing a second 'test filter' Γ and an additional small length scale $\delta < \ell$. A low-pass filtered velocity at scale δ was then defined by

$$\boldsymbol{u}^{>\delta}(\boldsymbol{x}) = \int \mathrm{d}^d \boldsymbol{r} \, \Gamma_\delta(\boldsymbol{r}) \boldsymbol{u}(\boldsymbol{x} + \boldsymbol{r}), \tag{3.1}$$

and likewise a stress contribution $\boldsymbol{\tau}^{>\delta}$, arising only from modes at length scales $> \delta$, by

$$\boldsymbol{\tau}^{>\delta} = \overline{\boldsymbol{u}^{>\delta}\boldsymbol{u}^{>\delta}} - \overline{\boldsymbol{u}^{>\delta}}\,\overline{\boldsymbol{u}^{>\delta}}. \tag{3.2}$$

The property of *ultraviolet (UV) locality* of the stress is that

$$\lim_{\delta \to 0} \boldsymbol{\tau}^{>\delta} = \boldsymbol{\tau}. \tag{3.3}$$

This limit means that modes at extreme subfilter scales ($\delta \ll \ell$) make little contribution to the stress at scale ℓ. The result (3.3) was proved in Eyink (2005), with convergence in a strong L^p-norm sense for any $p \geqslant 1$, under suitable spatial regularity assumptions on the velocity field. (In addition, some very mild moment-conditions must be satisfied by the filter kernels G and Γ; see Eyink 2005.) A sufficient condition is that the scaling exponent ζ_{2p} of the (absolute) $(2p)$th-order moment of the velocity-increment $\delta\boldsymbol{u}$ should satisfy the bound $\zeta_{2p} > 0$. There is also a similar property of *infrared (IR) locality*, which requires an oppposite condition $\zeta_{2p} < 2p$ (see Eyink 2005). However, we need not make use of IR locality in the present context.

3.1.1. *Multi-scale decomposition*

We can now reformulate the UV locality property as a multi-scale expansion of the stress tensor. First, we consider a corresponding multi-scale decomposition of the velocity field itself. Let us chose some parameter $\lambda < 1$, e.g. $\lambda = 2$ will be our standard choice. Then, consider a geometric sequence of lengths $\ell_n = \lambda^{-n}\ell$, for $n = 0, 1, 2, \ldots$. with $\ell_0 = \ell$ and $\ell_n \searrow 0$ as $n \to \infty$. For each of these we can define the corresponding low-pass filtered velocity field $\boldsymbol{u}^{(n)} = \boldsymbol{u}^{<\ell_n}$, or

$$\boldsymbol{u}^{(n)}(\boldsymbol{x}) = \int \mathrm{d}^d\boldsymbol{r}\ \Gamma_{\ell_n}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{x} + \boldsymbol{r}). \tag{3.4}$$

This field includes modes at all length-scales down to ℓ_n. We can also define a contribution to the velocity $\boldsymbol{u}^{[n]}$ that arises, roughly speaking, from the length-scales between ℓ_{n-1} and ℓ_n, by

$$\boldsymbol{u}^{[n]} = \boldsymbol{u}^{(n)} - \boldsymbol{u}^{(n-1)}, \quad n \geqslant 1. \tag{3.5}$$

It is convenient to set $\boldsymbol{u}^{[0]} = \boldsymbol{u}^{(0)}$. In that case, $\boldsymbol{u}^{(n)} = \sum_{k=0}^{n} \boldsymbol{u}^{[k]}$ for $n \geqslant 0$ and, taking the limit as $n \to \infty$, we obtain:

$$\boldsymbol{u} = \sum_{n=0}^{\infty} \boldsymbol{u}^{[n]}. \tag{3.6}$$

This is the multi-scale decomposition of the velocity field. It is closely related to other similar scale decompositions, such as multi-resolution expansions in wavelet bases, Paley–Littlewood decompositions, etc. Kraichnan (1974) used a multi-scale decomposition defined by banded Fourier series in order to discuss locality properties of the turbulent cascade. The series (3.6) will converge in an L^p norm, if, for example, the pth-order scaling exponent ζ_p of the absolute velocity increment $|\delta\boldsymbol{u}(\boldsymbol{r})|$ is positive. In fact, in that case, the series (3.6) has at least a geometric rate of convergence.

The scale locality proved in Eyink (2005) can be restated in the present terms by defining the stress $\boldsymbol{\tau}^{(n)} = \boldsymbol{\tau}^{>\ell_n}$, or

$$\boldsymbol{\tau}^{(n)} = \overline{\boldsymbol{u}^{(n)}\boldsymbol{u}^{(n)}} - \overline{\boldsymbol{u}^{(n)}}\,\overline{\boldsymbol{u}^{(n)}}, \tag{3.7}$$

which includes the contributions from all length scales $> \ell_n$. If we substitute the expansion $\boldsymbol{u}^{(n)} = \sum_{k=0}^{n} \boldsymbol{u}^{[k]}$ and take the limit $n \to \infty$, then we obtain a

doubly-infinite series

$$\boldsymbol{\tau} = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \boldsymbol{\tau}^{[n,n']}, \tag{3.8}$$

with $\boldsymbol{\tau}^{[n,n']} = \overline{\boldsymbol{u}^{[n]}\boldsymbol{u}^{[n']}} - \overline{\boldsymbol{u}^{[n]}}\ \overline{\boldsymbol{u}^{[n']}}$. This is the desired *multi-scale expansion of the stress tensor*. The term $\boldsymbol{\tau}^{[n,n']}$ represents a stress contribution from one velocity mode at length scale ℓ_n and another at length scale $\ell_{n'}$. The series (3.8) converges absolutely in the L^p-norm (and, in fact, at a geometric rate) under the same condition as mentioned in the UV locality statement, namely, the positivity of the scaling exponent of order $2p$, $\zeta_{2p} > 0$. This is a direct consequence of the concrete estimates in Eyink (2005).

A remark should be made concerning the limit $n \to \infty$ in the expansions (3.6) and (3.8). For a finite (but arbitrarily large) Reynolds number, this limit need not be taken, practically speaking, because the stress contribution from the scales below the dissipative microscale is negligibly small. Instead, the series can be truncated at some $n = n_d$ corresponding to the length scale of the viscous cutoff. However, for precisely this reason, there is also no difficulty in taking the limit $n \to \infty$ at a finite Reynolds number. In fact, the convergence rate of the expansion for n in the dissipation range of scales is greater than in the inertial range. As shown in Eyink (2005), the UV-locality of the stress depends upon the condition that the Hölder exponent of the velocity satisfies $\alpha > 0$, and, the larger α is, the better this property holds. Since the velocity field is smooth in the dissipation range ($\alpha = 1$), the UV-locality property is correspondingly stronger there than in the inertial range where $\alpha < 1$.

3.1.2. *Leading terms and strong UV-locality*

Truncation of the series (3.8) at its leading term corresponds to making a *strong UV-locality assumption*. In that case, the exact stress is approximated as

$$\boldsymbol{\tau} \approx \boldsymbol{\tau}^{[0,0]} = \overline{\boldsymbol{u}^{[0]}\boldsymbol{u}^{[0]}} - \overline{\boldsymbol{u}^{[0]}}\ \overline{\boldsymbol{u}^{[0]}}. \tag{3.9}$$

This approximation neglects all interactions with modes at subfilter lengths $< \ell_0 = \ell$. However, all interactions are retained between the modes at length scales above the filter scale (both scale-local and IR scale-non-local ones). This approximation achieves closure for the stress in terms of $\boldsymbol{u}^{[0]}$, essentially what is called the similarity model or Bardina model in the large-eddy simulation (LES) literature (Meneveau & Katz 2000). To simplify our discussion of this leading-order approximation, we may use a special notation for the low-pass filter of the velocity at scale ℓ with respect to the test kernel Γ, namely, $\widetilde{\boldsymbol{u}} = \Gamma_\ell \cdot \boldsymbol{u}$. Thus, $\widetilde{\boldsymbol{u}}$ and $\boldsymbol{u}^{[0]}$ are different notations for the same quantity. We introduce also a simplified notation for the complementary high-pass filter, $\boldsymbol{u}'' = \boldsymbol{u} - \widetilde{\boldsymbol{u}}$.

The approximation (3.9) is rather extreme and the results in Eyink (2005) show that subfilter scale modes can give a non-negligible contribution to the stress. Without repeating all the details from that work, we would like to consider briefly the magnitude of the error in making the strong UV-locality assumption. This approximation corresponds to replacing the exact velocity increment $\delta\boldsymbol{u}(r)$ in the formula (2.11) for the stress by $\delta\boldsymbol{u}^{(0)}(r) = \delta\widetilde{\boldsymbol{u}}(r)$. Let us assume that the velocity field has a Hölder exponent α, that is, $\delta\boldsymbol{u}(r) = O(r^\alpha)$ with $0 < \alpha < 1$. (This notation means, as usual, that there exists a constant A so that $|\delta\boldsymbol{u}(r)| \leqslant Ar^\alpha$, or, in a more dimensionally correct form, $|\delta\boldsymbol{u}(r)| \leqslant CU(r/L)^\alpha$, with L the integral length, U the r.m.s. velocity, and C a dimensionless constant.) Then, it is not hard to prove that $\boldsymbol{u}''(\boldsymbol{x}) = O(\ell^\alpha)$; see Eyink (2005) for details. An error of this magnitude is made for all $\boldsymbol{r}$ in replacing $\delta\boldsymbol{u}(r)$ by $\delta\widetilde{\boldsymbol{u}}(r)$. However, $\delta\boldsymbol{u}(r) = \delta\widetilde{\boldsymbol{u}}(r) + \delta\boldsymbol{u}''(r) = \delta\widetilde{\boldsymbol{u}}(r)[1 + O((\ell/r)^\alpha)] \approx \delta\widetilde{\boldsymbol{u}}(r)$ for

$r \gg \ell$. Therefore, the substitution of $\delta \widetilde{\boldsymbol{u}}(\boldsymbol{r})$ for $\delta \boldsymbol{u}(\boldsymbol{r})$ will be relatively accurate for increments over large separations $r \gg \ell$. Of course, this substitution will not be accurate in the opposite case of small separations, because $\widetilde{\boldsymbol{u}}$ is smooth and thus $\delta \widetilde{\boldsymbol{u}}(\boldsymbol{r}) \approx O(r) \ll \delta \boldsymbol{u}(\boldsymbol{r}) \approx O(r^\alpha)$ when $r \ll \ell$. Thus, a relatively large underestimate results when the strong UV-locality assumption is applied to velocity-increments at small separations.

Similar results hold for higher-order truncations, for example, for $\boldsymbol{\tau}^{(n)}$ defined by (3.7) with $n \geqslant 1$, or equivalently,

$$\boldsymbol{\tau} \approx \boldsymbol{\tau}^{(n)} = \sum_{k=0}^{n} \sum_{k'=0}^{n} \boldsymbol{\tau}^{[k,k']}. \tag{3.10}$$

This approximation assumes also UV-locality, but more weakly. It corresponds to replacing the exact velocity increment $\delta \boldsymbol{u}(\boldsymbol{r})$ in the formula (2.11) for the stress by $\delta \boldsymbol{u}^{(n)}(\boldsymbol{r})$, with an error $O(\ell_n^\alpha)$. This substitution will be relatively accurate when $r \gtrsim \ell_n$, but not for $r \lesssim \ell_n$. Here, let us note that (3.10) does not yield a closed formula in quite the same sense as does (3.9), since it involves all of the components $\boldsymbol{u}^{[k]}$ for $k = 0, \ldots, n$. If we assume that $G = \Gamma$, then $\boldsymbol{u}^{[0]} = \widetilde{\boldsymbol{u}} = \overline{\boldsymbol{u}}$. However, even if $G = \Gamma$, we cannot in general obtain the higher terms $\boldsymbol{u}^{[1]}, \ldots, \boldsymbol{u}^{[n]}$ uniquely from knowledge of $\overline{\boldsymbol{u}}$.

3.2. *Locality in space*

The turbulent stress is *a priori* non-local in space. The formula (2.11) expresses the stress as an average of velocity increments over separation vectors, which involves points, in principle, arbitrarily far away from the considered point. Nevertheless, the stress has some spatial locality properties, by virtue of the UV scale-locality discussed in the previous section. The latter property allows us to replace $\boldsymbol{u}$ by $\boldsymbol{u}^{(n)}$, with an error $O(\ell_n^\alpha)$ that becomes arbitrarily small for large enough n. The origin of the localness in space is then the smoothness of the filtered velocity field $\boldsymbol{u}^{(n)}$, which will be even analytic if the filter kernel Γ has a compactly supported Fourier transform. This smoothness allows us to represent filtered increments, such as $\delta \boldsymbol{u}^{(n)}(\boldsymbol{r})$, by a convergent Taylor expansion in the separation vector $\boldsymbol{r}$. The result is a formula that involves local gradients of the filtered velocities, i.e. velocity gradients at the point where the stress is to be evaluated.

3.2.1. *Gradient expansion*

Here we develop the gradient expansion for the stress, once contributions have been omitted from arbitrarily small scales. Let us first note the corresponding expansion of the filtered velocity $\boldsymbol{u}^{(n)}$ itself. This field is smooth and thus the Taylor polynomial of degree m,

$$\delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r};\boldsymbol{x}) = \sum_{p=1}^{m} \sum_{p_1+\cdots+p_d=p} \frac{r_1^{p_1} \cdots r_d^{p_d}}{p_1! \cdots p_d!} \left(\partial_1^{p_1} \cdots \partial_d^{p_d} \boldsymbol{u}^{(n)} \right)(\boldsymbol{x}) = \sum_{p=1}^{m} \frac{1}{p!} (\boldsymbol{r} \cdot \nabla)^p \boldsymbol{u}^{(n)}(\boldsymbol{x}), \tag{3.11}$$

converges to the increment $\delta \boldsymbol{u}^{(n)}(\boldsymbol{r};\boldsymbol{x})$ as $m \to \infty$. If the Taylor polynomial $\delta \boldsymbol{u}^{(n,m)}$ is substituted into (2.11), then it yields

$$\boldsymbol{\tau}^{(n,m)} = \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r}) \delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r}) - \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r}) \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r}), \tag{3.12}$$

which is our basic approximation to the stress.

An explicit expression is simplest to derive if we assume that the filter kernel G is spherically symmetric, as we shall do hereinafter. In that case, averages over the directions of the increment vector $\boldsymbol{r}$ can be evaluated by a standard formula for averages of a product of an even number of vector components over the unit sphere in d space dimensions. The result, which is easily proved by induction, is that

$$\int_{S^{d-1}} \varpi(d\boldsymbol{n}) n_{i_1} n_{i_2} \cdots n_{i_{2p-1}} n_{i_{2p}} = \frac{1}{d(d+2)\cdots[d+2(p-1)]} \sum_{\{i_1', i_1''\}, \ldots, \{i_p', i_p''\}} \delta_{i_1', i_1''} \cdots \delta_{i_p', i_p''}. \tag{3.13}$$

where summation is over all of the $(2p-1)!!$ pairings $\{i_1', i_1''\}, \ldots, \{i_p', i_p''\}$ of the $2p$ indices $i_1, i_2, \ldots, i_{2p-1}, i_{2p}$. An average of a product of an odd number of unit-vector components is equal to zero. Particular cases are for $p = 1$:

$$\int_{S^{d-1}} \varpi(d\boldsymbol{n}) n_i n_j = (1/d)\delta_{ij}, \tag{3.14}$$

and $p = 2$:

$$\int_{S^{d-1}} \varpi(d\boldsymbol{n}) n_i n_j n_k n_l = \frac{1}{d(d+2)} [\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}]. \tag{3.15}$$

We thus obtain a stress approximation for $m = 1$:

$$\tau_{ij}^{(n,1)} = \frac{C_2}{d} \ell^2 \frac{\partial u_i^{(n)}}{\partial x_k} \frac{\partial u_j^{(n)}}{\partial x_k}, \tag{3.16}$$

where $C_2 = \int d^d r\, G(\boldsymbol{r}) |\boldsymbol{r}|^2$ is the second-moment of the spherically symmetric filter function G. Likewise, for $m = 2$:

$$\tau_{ij}^{(n,2)} = \frac{C_2}{d} \ell^2 \frac{\partial u_i^{(n)}}{\partial x_k} \frac{\partial u_j^{(n)}}{\partial x_k} + \frac{C_4}{2d(d+2)} \ell^4 \frac{\partial^2 u_i^{(n)}}{\partial x_k \partial x_l} \frac{\partial^2 u_j^{(n)}}{\partial x_k \partial x_l}$$
$$+ \frac{dC_4 - (d+2)C_2^2}{4d^2(d+2)} \ell^4 \Delta u_i^{(n)} \Delta u_j^{(n)}, \tag{3.17}$$

where C_2 is as before and $C_4 = \int d^d r\, G(\boldsymbol{r}) |\boldsymbol{r}|^4$ is the fourth-moment of the spherically symmetric filter function G. In these expressions, we may further substitute the multi-scale decomposition $\boldsymbol{u}^{(n)} = \sum_{k=0}^{n} \boldsymbol{u}^{[k]}$ to obtain expansions such as for $m = 1$

$$\tau_{ij}^{(n,1)} = \frac{C_2}{d} \ell^2 \sum_{l=0}^{n} \sum_{l'=0}^{n} \frac{\partial u_i^{[l]}}{\partial x_k} \frac{\partial u_j^{[l']}}{\partial x_k}, \tag{3.18}$$

and similarly for $\boldsymbol{\tau}^{(n,m)}$ with $m > 1$. Thus, we obtain a *multi-scale gradient (MSG) expansion of the stress* simultaneously in scale and in space.

In Appendix A, we prove that $\boldsymbol{\tau}^{(n,m)}$ converges to $\boldsymbol{\tau}^{(n)}$ in the limit as $m \to \infty$. To keep the proof simple, we establish convergence in the spatial L^1-norm, requiring just finite energy for the velocity field $\boldsymbol{u}$. We assume also for the filter kernels that G decays faster than exponentially in space and that the Fourier transform $\widehat{\Gamma}$ has compact support. These specific assumptions can doubtless be modified in various ways, but they simplify the details of the proof. From our discussion of scale-locality in the preceding section, we recall that $\boldsymbol{\tau}^{(n)}$ also converges to $\boldsymbol{\tau}$ in the L^1-norm as $n \to \infty$, if the scaling exponent of the second-order structure function satisfies $\zeta_2 > 0$.

Thus, under these various assumptions, $\boldsymbol{\tau}^{(n,m)}$ converges in the L^1-norm to the exact stress $\boldsymbol{\tau}$ in the double limit taking first $m \to \infty$ and then $n \to \infty$.

It is rare to be able to show that a systematic turbulence approximation scheme is convergent. For example, Kraichnan (1970) has discussed previous attempts to construct expansion schemes based upon Reynolds number, where convergence has proved elusive. A case in point is the gradient expansion for the subscale stress proposed in Yeo & Bedford (1988), Leonard (1997) and Carati *et al.* (2001), based upon defiltering. As we discuss in Appendix B, there are many fluid velocity fields with finite energy – even infinitely smooth ones – for which the expansion (B 4) does not converge. The problem becomes more severe the more rapidly the Fourier transform of the filter kernel, $\widehat{G}(\boldsymbol{k})$, decays at large k. Our present study was motivated, in part, by the desire to overcome this difficulty. As we have shown (Appendix A and Eyink 2005), the multi-scale gradient expansion that we have elaborated does indeed converge, under realistic and rather mild conditions on the turbulent velocity field and with very modest regularity assumptions on the filter kernels. However, a price has been paid for this achievement. Unlike the expansion in Yeo & Bedford (1988), Leonard (1997) and Carati *et al.* (2001), our multi-scale gradient expansion is not closed in terms of the filtered field $\widetilde{\boldsymbol{u}} = \boldsymbol{u}^{[0]}$, but involves also the subscale fields $\boldsymbol{u}^{[1]}, \boldsymbol{u}^{[2]}, \ldots$. Thus, closure of our expansion requires an algorithm for estimating these unknown fields.

3.2.2. *Leading terms and strong space-locality*

Truncation of the gradient expansion $\boldsymbol{\tau}^{(n,m)}$ at small m values – e.g. approximating $\boldsymbol{\tau}^{(n)} \approx \boldsymbol{\tau}^{(n,1)}$ to first-order in gradients, as in (3.18) – corresponds to making a strong space-locality assumption. If the expansion is truncated also at small values of n, then both UV scale-locality and space-locality are assumed in a strong sense; for example setting $n = 0, m = 1$ gives

$$\tau_{ij}^{(0,1)} = \frac{C_2}{d} \ell^2 \frac{\partial \widetilde{u}_i}{\partial x_k} \frac{\partial \widetilde{u}_j}{\partial x_k}, \tag{3.19}$$

which is the standard first-order nonlinear model for the stress (Leonard 1974, 1997; Borue & Orszag 1998; Meneveau & Katz 2000). This observation gives some insight into the physical approximations underlying that model.

We would like to make an estimate of the error involved in truncating the gradient expansion to a given order m of space gradients. As in our discussion of scale-locality, we shall assume that the velocity field is Hölder continuous, so that $\delta \boldsymbol{u}(\boldsymbol{r}) = O(r^\alpha)$ for some $0 < \alpha < 1$. Then, it is not hard to show that the pth-order term in the Taylor expansion (3.11) of $\delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r})$ scales as $(\boldsymbol{r} \cdot \nabla)^p \boldsymbol{u}^{(n)} = O(\ell_n^\alpha (r/\ell_n)^p)$ for each $p \geqslant 1$ (e.g. see Eyink 2005). Compared with the exact increment $\delta \boldsymbol{u}(\boldsymbol{r})$, we see that each term is an underestimate for $r \lesssim \ell_n$ and an overestimate for $r \gtrsim \ell_n$, and the error is greater for larger p. Truncated to a given small order m, the Taylor approximation has the correct order of magnitude only for $r \approx \ell_n$. If we sum over all values of p, to infinite order in m, then we recover the approximation $\delta \boldsymbol{u}^{(n)}(\boldsymbol{r})$, which we have seen is an underestimate for $r \lesssim \ell_n$, but relatively accurate for $r \gtrsim \ell_n$.

Although this gradient expansion converges, there is no small parameter involved (except for $r \ll \ell_n$). The series (3.11) converges only because of the inverse factorials $1/p!$ that make coefficients of higher-order terms quite small. Thus, we can expect that very large values of m will be required to make $\delta \boldsymbol{u}^{(n,m)}(\boldsymbol{r}) \approx \delta \boldsymbol{u}^{(n)}(\boldsymbol{r}) \approx \delta \boldsymbol{u}(\boldsymbol{r})$ for $r \gg \ell_n$. Because the filter $G_\ell(\boldsymbol{r})$ is assumed to decay very rapidly, increments with $r \gg \ell$ give little contribution to the stress, and thus their poor approximation is not an issue.

However, increments for separations $\ell_n \lesssim r \lesssim \ell$ will give a significant contribution. In this interval, the effective expansion parameter, r/ℓ_n, takes values in the range from 1 for $r = \ell_n$ up to $\ell/\ell_n = \lambda^n$ for $r = \ell$. For small n, say $n = 0$ or 1, the expansion parameter is always $O(1)$ in the relevant interval of r, and the series converges quite rapidly. However, as n increases, the rate of convergence in m degrades rather quickly. A crude estimate of the size of m required for an accurate approximation is $m \gg \lambda^n$, in order for the terms $O(\lambda^{np}/p!)$ to be small for $p \approx m$. This estimate is probably too pessimistic, since it ignores cancellations that will occur in the average over r (cf. (3.13)). However, we can be sure that the m required to obtain $\boldsymbol{\tau}^{(n,m)} \approx \boldsymbol{\tau}^{(n)}$ will increase with increasing n.

4. The coherent-subregions approximation

We have proved that $\lim_{m\to\infty} \boldsymbol{\tau}^{(n,m)} = \boldsymbol{\tau}^{(n)}$, but also argued that larger orders of space gradients m are required to achieve this limit for increasing n. This stands to reason, because increasing the scale index n corresponds to adding finer small-scale structure to the velocity field. As the velocity field becomes rougher, higher-order terms in the spatial Taylor expansion become necessary in order to represent velocity increments accurately across fixed separations. On the other hand, even a first-order expansion of increments, $\delta \boldsymbol{u}^{(n)}(\boldsymbol{r}) \approx (\boldsymbol{r} \cdot \nabla)\boldsymbol{u}^{(n)}$, is correct on order of magnitude for separations $r \approx \ell_n$. Therefore, we should be able to obtain a reasonably accurate approximation by low-order gradients, if we use such expansions only for this range of separations where they are order-of-magnitude correct. In the present section, we shall use this strategy in order to construct an approximate multi-scale representation $\boldsymbol{\tau}_*^{(n,m)}$ for the turbulent stress. Although this modified expansion is no longer convergent to the exact stress, it may be more practically useful than the systematic approximation $\boldsymbol{\tau}^{(n,m)}$, because it should be more accurate for smaller orders m.

Although it turns out not to be the most serviceable approach, a natural first idea is to represent increments $\boldsymbol{r}$ of length $r \gg \ell_n$ as the sum of end-to-end increments across separations of length ℓ_n and then to Taylor expand each of the individual increments. Thus, defining the unit vector $\widehat{\boldsymbol{r}} = \boldsymbol{r}/r$, we could write

$$\delta \boldsymbol{u}^{(n)}(\boldsymbol{r}; \boldsymbol{x}) \approx \sum_{k=0}^{K} \delta \boldsymbol{u}^{(n)}(\ell_n \widehat{\boldsymbol{r}}; \boldsymbol{x} + k\ell_n \widehat{\boldsymbol{r}}) \approx \ell_n \sum_{k=0}^{K} (\widehat{\boldsymbol{r}} \cdot \nabla)\boldsymbol{u}^{(n)}(\boldsymbol{x} + k\ell_n \widehat{\boldsymbol{r}}), \qquad (4.1)$$

where K is the greatest integer less than or equal to r/ℓ_n. The formula (4.1) is likely to be fairly accurate, since the expansion parameter is $O(1)$ for each term in the sum. However, this expression involves velocity gradients evaluated at points $\boldsymbol{x} + k\ell_n \widehat{\boldsymbol{r}}$ on spheres of radius $k\ell_n$ about $\boldsymbol{x}$ for $k = 0, 1, \ldots, \lambda^n$ and spatially local expressions do not result for integrals over $\boldsymbol{r}$ when (4.1) is substituted into formula (2.11) for the stress. In order to obtain a simple local expression, we should instead Taylor-expand always about point $\boldsymbol{x}$. Thus, this approach does not lead to the desired result. However, at least it shows that an accurate representation of the stress is possible entirely in terms of filtered velocity gradients of low-order, although the representation is spatially non-local.

To obtain a local representation, we use Taylor expansions around $\boldsymbol{x}$, but only for displacements where they are both rapidly convergent and accurate. Let us decompose the integrals in (2.11) into contributions from 'shells'

$$\mathscr{S}_k = \{\boldsymbol{r} : \ell_{k-1} > |\boldsymbol{r}| > \ell_k\} \quad (k \geqslant 1). \qquad (4.2)$$
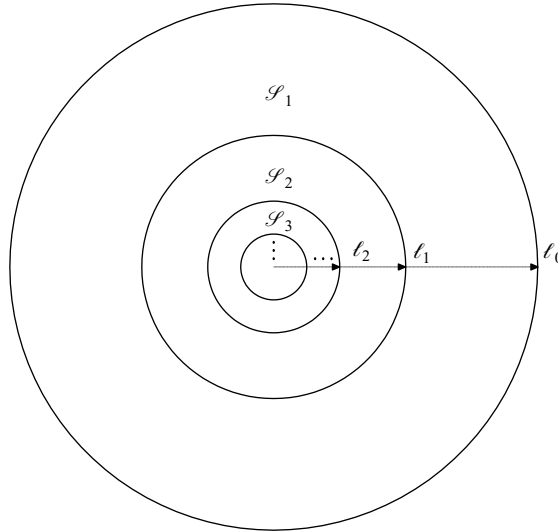
FIGURE 1. Shell decomposition of integration region. The figure illustrates the integration region over increment vectors in the stress formula (2.11). Most of the contribution comes from the ball of radius $\ell_0 = \ell$ around the point x. This ball is decomposed into 'shells' $\mathscr{S}_1, \mathscr{S}_2, \mathscr{S}_3, \ldots$. The Taylor expansion of the k-scale contribution to the stress is accurate and rapidly convergent in the shell $\mathscr{S}_k$. However, these shells have a smaller portion of the total volume as k increases.

See figure 1. Let us also define an 'outer shell'

$$\mathscr{S}_0 = \{r \,:\, |r| > \ell_0\} \tag{4.3}$$

and 'balls'

$$\mathscr{B}_k = \{r \,:\, |r| < \ell_{k-1}\} \quad (k \geqslant 1), \tag{4.4}$$

formed from unions of the 'shells' $\mathscr{S}_{k'}$ with $k' \geqslant k$. From our earlier discussion we expect that, for $r \in \mathscr{S}_k$,

$$\delta \boldsymbol{u}(r) \approx \delta \boldsymbol{u}^{[k]}(r) \approx \delta \boldsymbol{u}^{[k],(m)}(r), \tag{4.5}$$

for any Taylor polynomial of degree m, since the expansion parameter is here $r/\ell_k \approx 1$. Thus, we can obtain a rapidly convergent Taylor series expansion if we replace $\delta \boldsymbol{u}(r)$ by $\delta \boldsymbol{u}^{[k]}(r)$ for $r \in \mathscr{S}_k$. However, this replacement implies that modes at length scales $\leqslant \ell_k$ are now represented only for the increments with $r \in \mathscr{B}_k$. Furthermore, this ball $\mathscr{B}_k$ of radius ℓ_{k-1} occupies only a fraction $\sim \lambda^{-kd}$ of the total volume of the region $\mathscr{B}_1$ which effectively contributes to the stress. Therefore, such a replacement omits important subscale contributions to the stress. To compensate for this, we can use the calculated stress contribution from the shell $\mathscr{S}_k$ to estimate crudely the missing part, by multiplying the calculated contribution with an enhancement factor of $N_k = \lambda^{kd}$. This factor represents the number of subregions of volume $\sim \ell_k^d$ inside the ball $\mathscr{B}_1$ of radius ℓ. Multiplying each k-scale contribution in the shell $\mathscr{S}_k$ by the factor N_k amounts to the assumption that each of the subregions gives a similar or 'coherent' contribution to the stress. We shall therefore call this heuristic estimate the *coherent-subregions approximation (CSA)*. Let us proceed to develop it more systematically.

It is useful here to employ (2.12) which decomposes the stress into a 'systematic' part $\boldsymbol{\varrho}$ and a 'fluctuation' part $-\boldsymbol{u}'\boldsymbol{u}'$. These can be represented further by multiscale

decompositions

$$\varrho = \sum_{k=0}^{\infty} \sum_{k'=0}^{\infty} \varrho^{[k,k']}, \qquad \boldsymbol{u}' = \sum_{k=0}^{\infty} \boldsymbol{u}'^{[k]}, \tag{4.6}$$

analogous to (3.6), (3.8). Thus, $\varrho^{[k,k']}$ represents the contribution from one velocity mode at length scale ℓ_k and another at length scale $\ell_{k'}$. The multiscale decomposition of ϱ can be re-organized as

$$\varrho = \sum_{k=0}^{\infty} \varrho^{[k]}, \tag{4.7}$$

where

$$\varrho^{[k]} = \varrho^{[k,k]} + \sum_{l>k}^{\infty} \left\{ \varrho^{[k,l]} + \varrho^{[l,k]} \right\}. \tag{4.8}$$

The term $\varrho^{[k]}$ represents the contribution arising from a pair of modes, at least one at length scale ℓ_k and the second at an equal or smaller length scale. On the basis of these decompositions we can develop the desired approximation.

First, let us consider the 'systematic' part ϱ. The contributions $\varrho^{[k,k']}$ scale as $O(\ell_k^{\alpha} \ell_{k'}^{\alpha})$, when the velocity field has Hölder exponent α. It follows that the dominant term in $\varrho^{[k]}$ is the first one on the right-hand side of (4.8), or $\varrho^{[k,k]}$. It is possible that the remaining terms sum to a contribution of similar order. However, the first term, $\varrho^{[k,k]}$, is the average over space of positive-definite matrices, whereas the remaining terms have no definite sign and cancellations can be expected in the summation in (4.8). Thus, we expect that

$$\varrho^{[k]} \approx \varrho^{[k,k]} = \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{[k]}(\boldsymbol{r}) \delta \boldsymbol{u}^{[k]}(\boldsymbol{r}). \tag{4.9}$$

This motivates us to define the CSA value of $\varrho^{[k]}$, mth-order in gradients, as

$$\varrho_*^{[k],(m)} = N_k \int_{\mathscr{S}_k} \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{[k],(m)}(\boldsymbol{r}) \delta \boldsymbol{u}^{[k],(m)}(\boldsymbol{r}). \tag{4.10}$$

As discussed earlier, the factor N_k on the right-hand side of (4.10) corresponds to making the assumption that each subregion of $\mathscr{B}_1$ gives a contribution to the integral (4.9) similar to that of the kth 'shell' $\mathscr{S}_k$. This is reasonable, since the integrand is positive-definite and thus there will be little cancellation between the contributions from the different subregions, which can be expected to add together coherently. Using then the replacement (4.5) in the integral over $\mathscr{S}_k$ gives (4.10). As an additional argument in favour of the enhancement by N_k, let us note that $\varrho_*^{[k],(m)}$ defined in (4.10) with this factor gives an $O(\ell_k^{2\alpha})$ contribution to the stress, of the correct order of magnitude. See Appendix C.

Similar considerations apply also to the 'fluctuation' velocity $\boldsymbol{u}'$. The kth-scale contribution $\boldsymbol{u}'^{[k]}$ in (4.6) is written exactly as

$$\boldsymbol{u}'^{[k]} = - \int \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{[k]}(\boldsymbol{r}). \tag{4.11}$$

We then propose the CSA value of $\boldsymbol{u}'^{[k]}$, mth-order in gradients, as

$$\boldsymbol{u}_*'^{[k],(m)} = -N_k^{1/2} \int_{\mathscr{S}_k} \mathrm{d}^d \boldsymbol{r} \, G_\ell(\boldsymbol{r}) \delta \boldsymbol{u}^{[k],(m)}(\boldsymbol{r}). \tag{4.12}$$

Note the change in the enhancement factor to $N_k^{1/2}$. The integrand in (4.11) has no definite sign and the N_k different subregions should not be expected to contribute coherently. In a work on analytical closures, Kraichnan (1971) made a similar argument about the shear contribution from small scales, writing that 'random cancellation effects over the domain $1/k$ in linear dimension should reduce the effective shear of the high wavenumbers according to the $\sqrt{N}$ law.' Analogous reasoning motivates us to multiply the right-hand side of (4.12) by $N_k^{1/2}$.

This set of approximations altogether yields the *CSA-MSG expansion for the stress*, nth-order in scale index and mth-order in gradients:

$$\boldsymbol{\tau}_*^{(n,m)} = \sum_{k=0}^{n} \boldsymbol{\varrho}_*^{[k],(m)} - \sum_{k,k'=0}^{n} \boldsymbol{u}_*'^{[k],(m)} \boldsymbol{u}_*'^{[k'],(m)}, \tag{4.13}$$

Using the results for $m = 2$ as illustration, we can write

$$\boldsymbol{\varrho}_*^{[k],(2)} = \frac{\overline{C}_2^{[k]}}{d} \ell_k^2 \frac{\partial \boldsymbol{u}^{[k]}}{\partial x_l} \frac{\partial \boldsymbol{u}^{[k]}}{\partial x_l} + \frac{\overline{C}_4^{[k]}}{2d(d+2)} \ell_k^4 \frac{\partial^2 \boldsymbol{u}^{[k]}}{\partial x_l \partial x_m} \frac{\partial^2 \boldsymbol{u}^{[k]}}{\partial x_l \partial x_m}$$
$$+ \frac{\overline{C}_4^{[k]}}{4d(d+2)} \ell_k^4 \Delta \boldsymbol{u}^{[k]} \Delta \boldsymbol{u}^{[k]} \tag{4.14}$$

and

$$\boldsymbol{u}_*'^{[k],(2)} = \frac{1}{2d\sqrt{N_k}} \overline{C}_2^{[k]} \ell_k^2 \, \triangle \boldsymbol{u}^{[k]}. \tag{4.15}$$

As in (3.16), (3.17), we have used (3.13) in order to average over the directions of separation vectors $\boldsymbol{r}$ in (4.10), (4.12). Note that (4.14) has the same form as (3.17) for $\boldsymbol{\tau}^{(k,2)}$ except that the coefficients are different. The constants $\overline{C}_p^{[k]}$ for $p = 2, 4, \ldots$ are the partial pth moments of the kernel G over the kth 'shell' $\mathscr{S}_k$, multiplied by the factor $\lambda^{(d+p)k}$. Expressions are given for these constants in Appendix C, with G a Gaussian filter.

Our estimates are rough and are intended to be accurate qualitatively, but not more than order-of-magnitude accurate quantitatively. There is clearly ample room to improve the accuracy of the scheme, and many variants and refinements might be fruitfully considered. The basic approximation in the 'coherent-subregions' assumption, i.e. estimating missing small-scale contributions to the stress from their effects in subvolumes, will tend to enhance the level of fluctuations. However, the CSA stress $\boldsymbol{\tau}_*^{(n,m)}$ in (4.13) is still likely to be superior to the systematic MSG expansion $\boldsymbol{\tau}^{(n,m)}$ when $n \gtrsim 1$ and m is relatively small. The approximate stress $\boldsymbol{\tau}_*^{(n,m)}$ converges rapidly in the limit $m \to \infty$, to some value $\boldsymbol{\tau}_*^{(n)}$ which is, hopefully, a reasonable approximation of $\boldsymbol{\tau}^{(n)}$, requiring only moderately large values of m uniformly in n. It achieves our goal of providing a local expression for the stress which involves only filtered velocity gradients of low order. However, like $\boldsymbol{\tau}^{(n,m)}$, it is not a proper constitutive relation, because it is not closed in terms of $\widetilde{\boldsymbol{u}} = \boldsymbol{u}^{[0]}$. Of course, it already makes testable predictions for the stress, if the smaller-scale velocity fields $\boldsymbol{u}^{[k]}$ for $k \geqslant 1$ are determined from experiment or DNS and then substituted into the model. We report results of such a study elsewhere. Nevertheless, an *a priori* closure procedure would be useful for modelling purposes. This could be accomplished by a stochastic mapping which estimated the velocity gradients $\nabla \boldsymbol{u}^{[k]}, \nabla\nabla \boldsymbol{u}^{[k]}$, etc. for $k \geqslant 1$ from the corresponding gradients for $k = 0$. We hope to make this the subject of a future work.

5. The multi-scale gradient expansion in three dimensions

As an application of the general scheme, we shall consider here the turbulent cascades of energy and helicity in three space dimensions. In Eyink (2006), we discuss the MSG expansion of the stress for the inverse energy cascade in two space dimensions. Many other applications can be considered, such as turbulent vorticity transport in the two-dimensional enstrophy cascade (Eyink 2001; Chen *et al.* 2003*b*), or the turbulent stress tensor and electromotive force in three-dimensional magnetohydrodynamic cascades. The technical aspects of the expansion are similar in all of these cases. As we shall see in this section, our method yields a number of interesting predictions for the turbulent stress in three dimensions that may be tested either numerically or experimentally.

5.1. *The expansion of the turbulent stress*

We shall confine ourselves here to considering just the first-order ($m = 1$) term in the gradient expansion, or $\tau^{(n,1)}$ in (3.16). We have already noted that this first-order approximation is unlikely to be very accurate for larger n. On the other hand, because of the scale-locality of the energy cascade, only relatively small values of n need be considered and thus a first-order approximation may be adequate. Furthermore, except for the coefficient, $\tau^{(n,1)}$ has the same form as the term $\varrho_*^{[n],(m)}$ in (4.13) for $m = 1$:

$$\varrho_*^{[n],(1)} = \frac{\overline{C}_2^{[n]}}{d} \ell_n^2 \frac{\partial \boldsymbol{u}^{[n]}}{\partial x_l} \frac{\partial \boldsymbol{u}^{[n]}}{\partial x_l}, \tag{5.1}$$

and, in addition, the 'fluctuation' term in (4.13) vanishes for $m = 1$. Thus, the first-order CSA expansion has the closely similar form

$$\tau_*^{(n,1)} = \frac{1}{d} \sum_{k=0}^{n} \overline{C}_2^{[k]} \ell_k^2 \frac{\partial \boldsymbol{u}^{[k]}}{\partial x_l} \frac{\partial \boldsymbol{u}^{[k]}}{\partial x_l}. \tag{5.2}$$

We expect that $\tau_*^{(n,1)}$ in (5.2) for large n will be reasonably accurate in the three-dimensional inertial range. For example, the estimates in Appendix C show that the kth term in (5.2) scales $\sim O(\ell_k^{2\alpha})$ when the velocity field has Hölder exponent $0 < \alpha < 1$. This is the correct order of magnitude for the contribution to the stress from scale k and illustrates the UV locality of the stress. The series in (5.2) then converges at a geometric rate in the limit $n \to \infty$ and has the correct overall magnitude $\sim O(\ell^{2\alpha})$. By contrast, $\tau^{(n,1)}$ in (3.16) does not have the correct order of magnitude as $n \to \infty$, but is too large by a factor of $(\ell/\ell_n)^2$. This is due to an overestimate in $\tau^{(n,1)}$ of velocity-increments at large spatial separations, arising from the first-order Taylor expansion. Thus, our concrete results below for $\tau^{(n,1)}$ in three dimensions should be more properly reinterpreted, when n is large, for the approximation $\tau_*^{(n,1)}$ in (5.2) instead.

In any case, we have in three dimensions the formula for the filtered velocity gradient,

$$\frac{\partial u_i^{(n)}}{\partial x_j} = S_{ij}^{(n)} - \tfrac{1}{2} \epsilon_{ijk} \omega_k^{(n)}, \tag{5.3}$$

in terms of the filtered strain tensor $\boldsymbol{S}^{(n)}$, the filtered vorticity vector $\boldsymbol{\omega}^{(n)}$ and the antisymmetric Levi–Civita tensor ϵ_{ijk}. If (5.3) is substituted into (3.16), it yields

$$\tau_{ij}^{(n,1)} = \tfrac{1}{3} C_2 \ell^2 \left\{ S_{ik}^{(n)} S_{jk}^{(n)} + \tfrac{1}{2} \left[\left(\boldsymbol{\omega}^{(n)} \times \boldsymbol{S}^{(n)} \right)_{ij} + \left(\boldsymbol{\omega}^{(n)} \times \boldsymbol{S}^{(n)} \right)_{ji} \right] \right.$$
$$\left. + \tfrac{1}{4} \left(\delta_{ij} |\omega^{(n)}|^2 - \omega_i^{(n)} \omega_j^{(n)} \right) \right\}. \quad (5.4)$$

The separate terms in this expression have interesting physical interpretations. The first term is proportional to the strain-matrix squared:

$$\left[\boldsymbol{S}^{(n)} \right]^2 = \sum_{p=1}^{3} |\sigma_p^{(n)}|^2 \boldsymbol{e}_p^{(n)} \boldsymbol{e}_p^{(n)}, \quad (5.5)$$

where $\sigma_p^{(n)}$ and $\boldsymbol{e}_p^{(n)}$ are the eigenvalues and eigenvectors of the strain matrix $\boldsymbol{S}^{(n)}$, satisfying $\sigma_1^{(n)} + \sigma_2^{(n)} + \sigma_3^{(n)} = 0$. This term represents a tensile stress of magnitude $C_2 (\sigma_p^{(n)} \ell)^2 / 3$ exerted along each of the principal strain directions $\boldsymbol{e}_p^{(n)}$ for $p = 1, 2, 3$. The last term in (5.4) quadratic in the vorticity likewise represents a tensile stress along the two directions orthogonal to the filtered vorticity. However, the first part of that term proportional to the Kronecker delta function is an isotropic stress or turbulent pressure, which does not contribute to the deviatoric stress. The other half of the term, proportional to $\omega_i^{(n)} \omega_j^{(n)}$, is equivalent to a contractile stress of magnitude $-(1/12) C_2 (\omega^{(n)} \ell)^2$ exerted along vortex lines. Thus, one of the important effects of subscale modes is an induced tendency for lines of filtered vorticity $\boldsymbol{\omega}^{(n)}$ to resist lengthening. This 'elastic response' of vortex lines is well known in other contexts – for example, turbulence under rapid-distortion (Crow 1968). However, the most novel of the stress terms in (5.4) is the middle one, which is given by a certain 'cross-product' of strain and vorticity. More precisely, we have defined $(\boldsymbol{\omega}^{(n)} \times \boldsymbol{S}^{(n)})_{ij} = \epsilon_{ikl} \omega_k^{(n)} S_{lj}^{(n)}$. Note that this tensor is orthogonal to the strain at the same scale, $\boldsymbol{S}^{(n)} : (\boldsymbol{\omega}^{(n)} \times \boldsymbol{S}^{(n)}) = 0$, so that we call it the *skew-strain*. The middle term of (5.4), proportional to this skew-strain, is a sum of shear stresses,

$$\tfrac{1}{6} C_2 \sum_{p=1}^{3} \omega^{(n)} \sigma_p^{(n)} \sin \theta_p^{(n)} \left[\widetilde{\boldsymbol{e}}_p^{(n)} \boldsymbol{e}_p^{(n)} + \boldsymbol{e}_p^{(n)} \widetilde{\boldsymbol{e}}_p^{(n)} \right], \quad (5.6)$$

where $\theta_p^{(n)}$ is the angle between $\boldsymbol{\omega}^{(n)}$ and $\boldsymbol{e}_p^{(n)}$ and $\widetilde{\boldsymbol{e}}_p^{(n)}$ is the unit vector orthogonal to both $\boldsymbol{\omega}^{(n)}$ and $\boldsymbol{e}_p^{(n)}$, given by the right-hand rule. If we introduce the new unit vectors $\boldsymbol{e}_{p\pm}^{(n)} = [\boldsymbol{e}_p^{(n)} \pm \widetilde{\boldsymbol{e}}_p^{(n)}]/\sqrt{2}$, then (5.6) becomes

$$\tfrac{1}{6} C_2 \sum_{p=1}^{3} \omega^{(n)} \sigma_p^{(n)} \sin \theta_p^{(n)} \left[\boldsymbol{e}_{p+}^{(n)} \boldsymbol{e}_{p+}^{(n)} - \boldsymbol{e}_{p-}^{(n)} \boldsymbol{e}_{p-}^{(n)} \right]. \quad (5.7)$$

Hence, there are both tensile and contractile stresses exerted along the vectors $\boldsymbol{e}_{p\pm}^{(n)}$. These are obtained from the strain eigenvector $\boldsymbol{e}_p^{(n)}$ by rotating it $\pm\pi/4$ radians around the normal component of the vorticity vector $\boldsymbol{\omega}^{(n)}$.

The above vector formalism helps to make clear the geometry of the various stress contributions. However, it is perhaps more conventional to write these stresses in terms of the fluid deformation matrix $\boldsymbol{D}^{(n)}$, defined by $D_{ij}^{(n)} = \partial u_i^{(n)} / \partial x_j$, and its symmetric part $\boldsymbol{S}^{(n)}$ and antisymmetric part $\boldsymbol{\Omega}^{(n)}$. Of course, $\boldsymbol{S}^{(n)}$ is the strain tensor and $\boldsymbol{\Omega}^{(n)}$ is related to the vorticity vector $\boldsymbol{\omega}^{(n)}$ by the standard relation $\Omega_{ij}^{(n)} = -\epsilon_{ijk} \omega_k^{(n)} / 2$. In terms of the deformation matrix the first-order term (3.16) in the MSG expansion can be written (in fact, in any dimension d) as

$$\boldsymbol{\tau}^{(n,1)} = \frac{1}{d} C_2 \ell^2 \boldsymbol{D}^{(n)} \left[\boldsymbol{D}^{(n)} \right]^\top. \quad (5.8)$$

The decomposition analogous to (5.4) is then

$$\boldsymbol{\tau}^{(n,1)} = \frac{1}{d}C_2\ell^2\big\{\boldsymbol{S}^{(n)}\boldsymbol{S}^{(n)} + \big[\boldsymbol{\Omega}^{(n)}, \boldsymbol{S}^{(n)}\big] - \boldsymbol{\Omega}^{(n)}\boldsymbol{\Omega}^{(n)}\big\}, \tag{5.9}$$

where $[\boldsymbol{\Omega}^{(n)}, \boldsymbol{S}^{(n)}] = \boldsymbol{\Omega}^{(n)}\boldsymbol{S}^{(n)} - \boldsymbol{S}^{(n)}\boldsymbol{\Omega}^{(n)}$ is the commutator matrix. Thus, in three dimensions, $\boldsymbol{S}^{(n)}\boldsymbol{S}^{(n)}$ is the strain-squared as in (5.5), $-\boldsymbol{\Omega}^{(n)}\boldsymbol{\Omega}^{(n)}$ gives the tensile stress in the plane normal to vortex lines, and $[\boldsymbol{\Omega}^{(n)}, \boldsymbol{S}^{(n)}]$ is the 'skew-strain'.

5.2. *Energy cascade in three dimensions*

Consider the consequences of the stress in formula (5.4) for the energy cascade. When (5.4) is substituted into equation (2.8) for the energy flux, we obtain the following result to first-order in gradients:

$$\Pi^{(n,1)} = \tfrac{1}{3}C_2\ell^2\big\{ -\mathrm{Tr}\,\big(\overline{\boldsymbol{S}}(\boldsymbol{S}^{(n)})^2\big) + \tfrac{1}{4}\big(\boldsymbol{\omega}^{(n)}\big)^\top \overline{\boldsymbol{S}}\big(\boldsymbol{\omega}^{(n)}\big) + \overline{\boldsymbol{S}}:\big(\boldsymbol{S}^{(n)}\times\boldsymbol{\omega}^{(n)}\big)\big\}. \tag{5.10}$$

The middle term has an obvious physical meaning. It represents the rate of work done by the filtered strain $\overline{\boldsymbol{S}}$ in order to stretch the lines of vorticity $\boldsymbol{\omega}^{(n)}$ against the resisting contractile stress of the subscales. This remarkable relationship between energy flux and *vortex stretching* was observed by Borue & Orszag (1998) using the nonlinear model, which is a special case of our result for $n = 0$ and $G = \Gamma$:

$$\Pi^{(0,1)} = \tfrac{1}{3}C_2\ell^2\big\{-\mathrm{Tr}\,\big(\overline{\boldsymbol{S}}^3\big) + \tfrac{1}{4}\overline{\boldsymbol{\omega}}^\top \overline{\boldsymbol{S}}\,\overline{\boldsymbol{\omega}}\big\}. \tag{5.11}$$

Vortex stretching was suggested by Taylor (1938) as the basic dissipation mechanism of three-dimensional turbulence. Note that the first term in (5.11) proportional to the *strain skewness* can also be related to vortex stretching, on average, using a relation of Betchov (1956). His result states that for an incompressible fluid $-\langle\mathrm{Tr}\,(\overline{\boldsymbol{S}}^3)\rangle = (3/4)\langle\overline{\boldsymbol{\omega}}^\top \overline{\boldsymbol{S}}\,\overline{\boldsymbol{\omega}}\rangle$, where $\langle\cdot\rangle$ denotes either ensemble average over a statistically homogeneous turbulence or any volume average where boundary terms from integration-by-parts can be ignored. According to Betchov's relation, precisely 75 % of the mean energy flux in the nonlinear model comes from strain skewness and 25 % from vortex stretching. Betchov's relation can be generalized as follows:

$$-\big\langle\mathrm{Tr}\big(\overline{\boldsymbol{S}}\big(\boldsymbol{S}^{(n)}\big)^2\big)\big\rangle = \tfrac{1}{2}\big\langle(\overline{\boldsymbol{\omega}})^\top \boldsymbol{S}^{(n)}\big(\boldsymbol{\omega}^{(n)}\big)\big\rangle + \tfrac{1}{4}\big\langle\big(\boldsymbol{\omega}^{(n)}\big)^\top \overline{\boldsymbol{S}}\big(\boldsymbol{\omega}^{(n)}\big)\big\rangle. \tag{5.12}$$

This result is proved in our Appendix D under the same assumptions as Betchov's. By using (5.12), the first term in (5.10) can be related to vortex stretching in general for all n. However, the last term in (5.10) appears to be fundamentally different. It appears only due to contributions of subscales and there is no analogue in the nonlinear model (5.11) for $n = 0$. Some additional insight on that term can be obtained by rewriting $\overline{\boldsymbol{S}}:(\boldsymbol{S}^{(n)}\times\boldsymbol{\omega}^{(n)}) = \boldsymbol{\omega}^{(n)}\cdot(\overline{\boldsymbol{S}}\times\boldsymbol{S}^{(n)})$, where $\overline{\boldsymbol{S}}\times\boldsymbol{S}^{(n)}$ is the dual vector corresponding to the antisymmetric commutator matrix $[\overline{\boldsymbol{S}}, \boldsymbol{S}^{(n)}]$, i.e. $(\overline{\boldsymbol{S}}\times\boldsymbol{S}^{(n)})_i = (1/2)\varepsilon_{ijk}([\overline{\boldsymbol{S}}, \boldsymbol{S}^{(n)}])_{jk}$. Thus, this new term arises from rotation of the subscale strain $\boldsymbol{S}^{(n)}$ relative to the filtered strain $\overline{\boldsymbol{S}}$, and vanishes if the orthogonal eigenframes of these two symmetric matrices coincide.

Using the CSA stress in (5.2), we obtain a result similar to (5.10):

$$\Pi_*^{(n,1)} = \tfrac{1}{3}\sum_{k=0}^{n}\overline{C}_2^{[k]}\ell_k^2\big\{-\mathrm{Tr}\,\big(\overline{\boldsymbol{S}}(\boldsymbol{S}^{[k]})^2\big) + \tfrac{1}{4}\big(\boldsymbol{\omega}^{[k]}\big)^\top \overline{\boldsymbol{S}}\big(\boldsymbol{\omega}^{[k]}\big) + \overline{\boldsymbol{S}}:\big(\boldsymbol{S}^{[k]}\times\boldsymbol{\omega}^{[k]}\big)\big\}. \tag{5.13}$$

The remarks we have made above on physical interpretation of $\Pi^{(n,1)}$ apply equally here. However, the sum in (5.13) also has a limit for large n and we expect that it gives

a quite reasonable model for energy flux in three dimensions. Using the generalized Betchov relation (5.12), the CSA mean flux can be written as

$$\langle \Pi_*^{(n,1)} \rangle = \tfrac{1}{3} \sum_{k=0}^{n} \overline{C}_2^{[k]} \ell_k^2 \{ \tfrac{1}{2} \langle (\overline{\boldsymbol{\omega}})^\top \boldsymbol{S}^{[k]} (\boldsymbol{\omega}^{[k]}) \rangle + \tfrac{1}{2} \langle (\boldsymbol{\omega}^{[k]})^\top \overline{\boldsymbol{S}} (\boldsymbol{\omega}^{[k]}) \rangle + \langle \overline{\boldsymbol{S}} : (\boldsymbol{S}^{[k]} \times \boldsymbol{\omega}^{[k]}) \rangle \}. \tag{5.14}$$

The first two terms in each summand arise from vortex stretching and will tend to be positive, certainly for small k when $\boldsymbol{S}^{[k]} \propto \overline{\boldsymbol{S}}$, $\boldsymbol{\omega}^{[k]} \propto \overline{\boldsymbol{\omega}}$. On the other hand, the third term from skew-strain then nearly vanishes. For the latter term to be important, there must be some characteristic rotation of $\boldsymbol{S}^{[k]}$ relative to $\overline{\boldsymbol{S}}$ as k increases. Of course, it is not hard to see that each term is zero on average when $\boldsymbol{S}^{[k]}$, $\boldsymbol{\omega}^{[k]}$ are uncorrelated with $\overline{\boldsymbol{S}}$, which must be expected in the limit as $k \to \infty$. Therefore, it is only for intermediate values of k that the third term can contribute to mean energy flux.

The physical mechanism of energy cascade by these stress terms can be illustrated by the following:

EXAMPLE 1. *Vortex tube stretched by a constant strain*

We consider a small-scale cylindrical vortex tube, parallel to the z-axis, with circular cross-section of radius $R = \ell_k$ and with vorticity magnitude $\omega_0 = \omega^{[k]}$. This is an exact stationary solution of the three-dimensional Euler equation with two-dimensional symmetry. Thus, it may be described by a pseudoscalar streamfunction

$$\psi^{[k]}(x, y) = \begin{cases} \tfrac{1}{4} \omega_0 [R^2 - r^2], & r < R, \\ -\tfrac{1}{2} \omega_0 R^2 \ln(r/R), & r > R, \end{cases} \tag{5.15}$$

where r is the radial distance from the z-axis in cylindrical coordinates (r, θ, z). The corresponding velocity field is

$$\boldsymbol{u}^{[k]}(x, y) = \begin{cases} \tfrac{1}{2} \omega_0 \widehat{z} \times \boldsymbol{r}, & r < R, \\ \tfrac{1}{2} \omega_0 (R/r)^2 \widehat{z} \times \boldsymbol{r}, & r > R, \end{cases} \tag{5.16}$$

where $\widehat{z}$ is the unit vector in the z-direction (see figure 2). This small-scale field is now superimposed with a large-scale velocity

$$\overline{\boldsymbol{u}} = \begin{bmatrix} -(\overline{\sigma}/2)x \\ -(\overline{\sigma}/2)y \\ \overline{\sigma}z \end{bmatrix}, \tag{5.17}$$

with deformation matrix $\overline{\boldsymbol{D}}$

$$\overline{\boldsymbol{D}} = \begin{bmatrix} -\overline{\sigma}/2 & 0 & 0 \\ 0 & -\overline{\sigma}/2 & 0 \\ 0 & 0 & \overline{\sigma} \end{bmatrix}. \tag{5.18}$$

This is a pure large-scale strain $\overline{\boldsymbol{D}} = \overline{\boldsymbol{S}}$ with vorticity $\overline{\boldsymbol{\omega}} = \boldsymbol{o}$. If $\overline{\sigma} > 0$, then this corresponds to an axisymmetric stretching along the z-direction and compression in the other two directions (figure 2). The combination of the large-scale and small-scale fields gives an exact solution of the three-dimensional Euler equation $(\partial_t + \boldsymbol{u} \cdot \nabla) \boldsymbol{\omega}^{[k]}(t) = (\boldsymbol{\omega}^{[k]}(t) \cdot \nabla) \boldsymbol{u} = 0$, where $\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}^{[k]}(t)$ and where $\boldsymbol{\omega}^{[k]}(t)$ is the same as the initial vorticity field, made time-dependent by the substitutions $\omega(t) = e^{\overline{\sigma}t} \omega_0$ and $R(t) = e^{-\overline{\sigma}t/2} R$. For example, see Neu (1984), who considers a more general set of
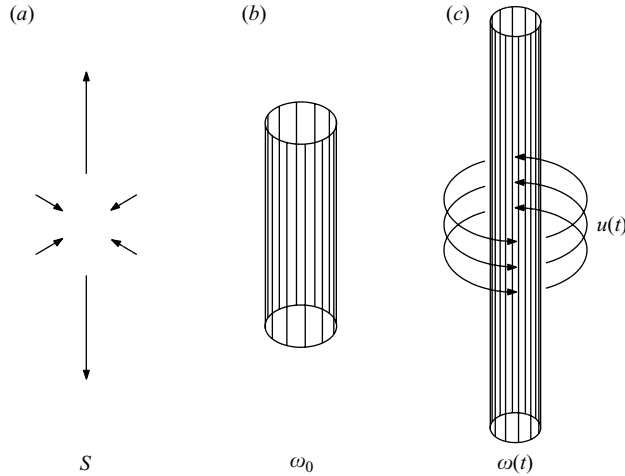
FIGURE 2. Energy cascade by vortex-stretching. (*b*) A cylindrical tube of parallel vortex lines in (*a*) a constant strain field with stretching direction along the vortex axis. (*c*) The result is that the vortex is stretched and its cross-sectional area shrunken. The 'spin-up' of the vortex increases its energy and generates more positive (tensile) stress in the plane perpendicular to the vortex axis.

solutions. In the present case, the small-scale vortex is stretched along its axis and, by incompressibility, its cross-section shrinks. To conserve the circulation around the tube, the vorticity and the velocity in the small scales correspondingly increase (see figure 2). This 'spin-up' by the large-scale strain results in a transfer of energy to the small scales.

The process can be understood from our general formulae above. Without loss of generality, we can focus on the instantaneous transfer at the initial time $t = 0$. The velocity-gradient tensor in the small scales is then

$$D^{[k]}(x, y) = \begin{cases} \frac{1}{2}\omega^{[k]} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & r < \ell_k, \\ \frac{1}{2}\omega^{[k]} \left(\frac{\ell_k}{r}\right)^2 \begin{bmatrix} \sin(2\theta) & -\cos(2\theta) & 0 \\ -\cos(2\theta) & -\sin(2\theta) & 0 \\ 0 & 0 & 0 \end{bmatrix}, & r > \ell_k. \end{cases} \tag{5.19}$$

This is purely rotational for $r < \ell_k$ and is a pure strain for $r > \ell_k$. Substituting into (5.1) gives the stress

$$\tau_*^{[k],(1)} = \frac{1}{12}\overline{C}^{[k]}|\omega^{[k]}\ell_k|^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times \begin{cases} 1, & r < \ell_k, \\ (\ell_k/r)^4, & r > \ell_k, \end{cases} \tag{5.20}$$

to first order in gradients. This result represents the $-\Omega^{[k]}\Omega^{[k]}$ term for $r > \ell_k$ and the $S^{[k]}S^{[k]}$ term for $r > \ell_k$. The 'skew-strain' vanishes identically for this right cylindrical vortex tube. We see that the net stress is tensile in the two-dimensional plane perpendicular to the vortex tube, set up by the velocity circulating around the vortex axis. Its deviatoric part includes a contractile stress along the vortex axis. These stresses oppose the axial stretching and lateral compression by the large-scale strain, and increase in magnitude as the vortex spins up. The work of the large-scale

strain against these resistive stresses is the basic mechanism of energy transfer to the small scales.

If $\overline{\sigma} < 0$, then the energy flux corresponding to (5.20)

$$\Pi_*^{[k],(1)} = \tfrac{1}{12}\overline{C}^{[k]}\overline{\sigma}\big|\omega^{[k]}\ell_k\big|^2 \times \begin{cases} 1, & r < \ell_k, \\ (\ell_k/r)^4, & r > \ell_k, \end{cases} \tag{5.21}$$

is negative and the large-scale strain 'spins down' the small-scale vortex, by the time-reverse of the process considered above. What is crucial for foward energy transfer is that the vortex should align with a stretching direction of the large-scale strain rather than with a shrinking direction. We know from the relation of Betchov (1956) that, in an incompressible flow, mean vortex-stretching requires that there be typically two positive strain eigenvalues and one negative eigenvalue. This tendency has been confirmed for dissipation-range velocity gradients by DNS (Ashurst *et al.* 1987) and for inertial-range (filtered) velocity gradients by experiment (Tao, Katz & Meneveau 2002; Van der Bos *et al.* 2002). Furthermore, these empirical studies have shown that the vorticity vector tends to align with the intermediate weakly stretching eigendirection of the strain at the same scale, rather than with the strongest stretching direction. Some theoretical understanding of how this occurs can be obtained from simple Lagrangian dynamical models of the velocity gradients (Vieillefosse 1982, 1984; Cantwell 1992; Chertkov, Pumir & Shraiman 1999). Thus, the situation in turbulence is slightly different from that which we imagined in our simple example above. However, the mechanism of the energy transfer process appears to be essentially the same.

5.3. *Helicity cascade in three dimensions*

It is well-known that three-dimensional smooth solutions of the inviscid, incompressible fluid equations have in addition to the energy a second quadratic invariant, the helicity (Moreau 1961; Moffatt 1969):

$$H(t) = \int \mathrm{d}^3 x\, u(x, t) \cdot \omega(x, t). \tag{5.22}$$

When helicity is input at large scales together with energy, then there is in three dimensions a joint cascade of both invariants to high-wavenumber (Brissaud *et al.* 1973; Kraichnan 1973). The flux of helicity can be expressed quite similarly to the flux of energy in (2.7), as

$$\Lambda = -2\nabla\overline{\omega} : \tau. \tag{5.23}$$

See Chen, Chen & Eyink (2003*a*). Equation (5.23) implies that the stress τ must be correlated simultaneously with both the velocity gradient and the vorticity gradient in a joint cascade of energy and helicity. Our work sheds some light on how this is achieved.

A vorticity gradient may be decomposed into symmetric and antisymmetric parts, as:

$$\frac{\partial \omega_i}{\partial x_j} = R_{ij} + \Xi_{ij} = R_{ij} - \tfrac{1}{2}\epsilon_{ijk}\xi_k, \tag{5.24}$$

where $\mathbf{R} = (1/2)[(\nabla\omega) + (\nabla\omega)^\top]$, $\mathbf{\Xi} = (1/2)[(\nabla\omega) - (\nabla\omega)^\top]$ and $\mathbf{\xi} = \nabla\times\omega$. We may write the helicity flux also as $\Lambda = -2\overline{\mathbf{R}} : \tau$, because of the symmetry of the stress tensor. Therefore, if we substitute the first-order stress formula (5.4), then we obtain

the expression for helicity flux analogous to (5.10):

$$\Lambda^{(n,1)} = \tfrac{2}{3}C_2\ell^2 \left\{ -\text{Tr}\left(\overline{\boldsymbol{R}}(\boldsymbol{S}^{(n)})^2\right) + \tfrac{1}{4}(\boldsymbol{\omega}^{(n)})^\top \overline{\boldsymbol{R}}(\boldsymbol{\omega}^{(n)}) + \overline{\boldsymbol{R}} : (\boldsymbol{S}^{(n)} \times \boldsymbol{\omega}^{(n)}) \right\}. \qquad (5.25)$$

This is the exact expression to first-order in gradients. Of course, we can also write down a CSA expansion for helicity flux,

$$\Lambda_*^{(n,1)} = \tfrac{2}{3} \sum_{k=0}^{n} \overline{C}_2^{[k]} \ell_k^2 \left\{ -\text{Tr}\left(\overline{\boldsymbol{R}}(\boldsymbol{S}^{[k]})^2\right) + \tfrac{1}{4}(\boldsymbol{\omega}^{[k]})^\top \overline{\boldsymbol{R}}(\boldsymbol{\omega}^{[k]}) + \overline{\boldsymbol{R}} : (\boldsymbol{S}^{[k]} \times \boldsymbol{\omega}^{[k]}) \right\}, \quad (5.26)$$

analogous to (5.13) for energy flux. All the stress components – from strain-squared, from vortex contraction, and from skew-strain – contribute to the helicity flux. Note that the generalized Betchov relation from Appendix D can be applied to give

$$-\left\langle \text{Tr}\left(\overline{\boldsymbol{R}}(\boldsymbol{S}^{[k]})^2\right)\right\rangle = \tfrac{1}{2}\langle \overline{\boldsymbol{\xi}}^\top \boldsymbol{S}^{[k]} \boldsymbol{\omega}^{[k]} \rangle + \tfrac{1}{4}\langle (\boldsymbol{\omega}^{[k]})^\top \overline{\boldsymbol{R}} \boldsymbol{\omega}^{[k]} \rangle, \qquad (5.27)$$

where $\langle \cdot \rangle$ denotes a homogeneous average. Thus, the strain-squared contribution can be replaced on average with the above two terms.

It is known that the helicity cascade is local in scale (Eyink 2005). Therefore, it is interesting to consider the $n = 0$ contribution, which, assuming $G = \Gamma$, coincides with the helicity flux for the nonlinear model of the stress. Now, it is not hard to see that

$$\overline{\boldsymbol{\omega}}^\top \overline{\boldsymbol{R}} \overline{\boldsymbol{\omega}} = \nabla \cdot \left[\tfrac{1}{2}|\overline{\boldsymbol{\omega}}|^2 \overline{\boldsymbol{\omega}} \right], \qquad (5.28)$$

which is a total derivative. Thus,

$$\tfrac{1}{4}\langle \overline{\boldsymbol{\omega}}^\top \overline{\boldsymbol{R}} \overline{\boldsymbol{\omega}} \rangle = 0, \qquad (5.29)$$

and the contractile stress along vortex lines gives no contribution to the UV-local part of mean helicity flux. Combining (5.29) and the generalized Betchov relation (5.27) gives also

$$-\langle \text{Tr}\left(\overline{\boldsymbol{R}}(\overline{\boldsymbol{S}})^2\right)\rangle = \tfrac{1}{2}\langle \overline{\boldsymbol{\xi}}^\top \overline{\boldsymbol{S}} \overline{\boldsymbol{\omega}} \rangle. \qquad (5.30)$$

Therefore, the total UV-local ($n = 0$) contribution to mean helicity flux is

$$\langle \Lambda^{(0,1)} \rangle = \tfrac{2}{3}C_2\ell^2 \left\{ \tfrac{1}{2}\langle \overline{\boldsymbol{\xi}}^\top \overline{\boldsymbol{S}} \overline{\boldsymbol{\omega}} \rangle + \langle \overline{\boldsymbol{R}} : (\overline{\boldsymbol{S}} \times \overline{\boldsymbol{\omega}}) \rangle \right\}. \qquad (5.31)$$

Equivalently, this is the nonlinear model expression for mean helicity flux. The first term arises from the stress proportional to strain-squared and the second term from the stress proportional to skew-strain.

The two terms in (5.31) can be related by the following identity

$$\tfrac{1}{2}\overline{\boldsymbol{\xi}}^\top \overline{\boldsymbol{S}} \overline{\boldsymbol{\omega}} = -\overline{\boldsymbol{\varXi}} : (\overline{\boldsymbol{S}} \times \overline{\boldsymbol{\omega}}). \qquad (5.32)$$

This is easily proved by substituting on the right $\overline{\varXi}_{ij} = -(1/2)\epsilon_{ijk}\overline{\xi}_k$, then using the definition of the skew-strain and the identity $\epsilon_{mij}\epsilon_{mkl} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$. Since $(\nabla \overline{\boldsymbol{\omega}})^\top = \overline{\boldsymbol{R}} - \overline{\boldsymbol{\varXi}}$, using (5.32) in (5.31) gives

$$\langle \Lambda^{(0,1)} \rangle = \tfrac{2}{3}C_2\ell^2 \langle (\nabla \overline{\boldsymbol{\omega}})^\top : (\overline{\boldsymbol{S}} \times \overline{\boldsymbol{\omega}}) \rangle. \qquad (5.33)$$

Thus we see that both the symmetric and antisymmetric parts of the vorticity gradient can contribute to helicity flux. The result (5.33) also makes clear the important role of the skew-strain in the three-dimensional helicity cascade. It is noteworthy that skew-strain makes no UV-local contribution to energy flux at all and is thus free to adjust as necessary to maintain the helicity flux in a joint cascade of both invariants.

If we use the result $(1/2)\overline{\boldsymbol{\xi}}^{\top}\mathbf{S}^{[k]}\boldsymbol{\omega}^{[k]} = -\overline{\boldsymbol{\Xi}}:(\mathbf{S}^{[k]}\times\boldsymbol{\omega}^{[k]})$ analogous to (5.32), the generalized Betchov relation (5.27), and the expression (5.26), then we obtain

$$\langle \Lambda_*^{(n,1)}\rangle = \tfrac{2}{3}\sum_{k=0}^{n}\overline{C}_2^{[k]}\ell_k^2\{\langle(\nabla\overline{\boldsymbol{\omega}})^{\top}:(\mathbf{S}^{[k]}\times\boldsymbol{\omega}^{[k]})\rangle + \tfrac{1}{2}\langle(\boldsymbol{\omega}^{[k]})^{\top}\overline{\mathbf{R}}(\boldsymbol{\omega}^{[k]})\rangle\},\tag{5.34}$$

for the CSA expansion of mean helicity flux. This is analogous to the similar result (5.14) for the mean energy flux. However, note that it is now the first term which makes a UV-local contribution while the second only contributes for intermediate values of k.

We now consider a simple example to illustrate the mechanism of helicity cascade by these stress terms:

EXAMPLE 2. *Vortex tube twisted by a constant screw*

We take as our model of the small scales an exact stationary solution of three-dimensional Euler equations which was previously considered by Moffatt (1969) as an example of a helical flow with continuous vorticity distribution. It is a two-dimensional but three-component velocity field, closely related to our Example 1. Indeed, the horizontal components $(u^{[k]}, v^{[k]})$ of the velocity field are the same as those in (5.16), obtained from the two-dimensional streamfunction $\psi^{[k]}$ in (5.15). However, this is now supplemented with a vertical velocity component

$$w^{[k]}(x,y) = \begin{cases} \tfrac{1}{4}\omega_0 p[R^2 - r^2], & r < R, \\ 0, & r > R. \end{cases}\tag{5.35}$$

It can easily be shown that the resulting total velocity field is a stationary Euler solution (e.g. see Moffatt 1969, §6(a).) If $p = 0$, then this solution coincides with that in our Example 1. The meaning of the parameter p can best be understood by considering the associated vorticity vector $\boldsymbol{\omega}^{[k]} = (\alpha^{[k]}, \beta^{[k]}, \gamma^{[k]})$. Of course, the vertical component $\gamma^{[k]}$ is the same as in Example 1, $\gamma^{[k]} = \omega_0$ for $r < R$ and $\gamma^{[k]} = 0$ for $r > R$. The horizontal components are obtained using the vertical velocity as a 'streamfunction':

$$\begin{bmatrix}\alpha^{[k]} \\ \beta^{[k]}\end{bmatrix} = \begin{bmatrix}\partial w^{[k]}/\partial y \\ -\partial w^{[k]}/\partial x\end{bmatrix} = \tfrac{1}{2}\omega_0 p\begin{bmatrix}-y \\ x\end{bmatrix},\tag{5.36}$$

for $r < R$ and is equal to 0 for $r > R$. The vortex lines are helices winding around the z-axis with 'pitch' $4\pi/p$, i.e. making one counterclockwise revolution in that vertical distance. It is not hard to check that the solution given by (5.15), (5.16), (5.35) and (5.36) has a constant helicity density $h^{[k]} = \boldsymbol{u}^{[k]}\cdot\boldsymbol{\omega}^{[k]} = (1/4)\omega_0^2 R^2 p$ for $r < R$ and is equal to 0 for $r > R$.

We shall take as our model of the large scales the velocity

$$\overline{\boldsymbol{u}} = \begin{bmatrix}-\overline{\rho}yz/2 \\ \overline{\rho}xz/2 \\ 0\end{bmatrix}.\tag{5.37}$$

This corresponds to a constant *screw*, i.e. solid-body rotation in each plane parallel to the (x, y)-plane with an angular velocity $\overline{\rho}z/2$ that grows linearly in z. It is a right-hand screw for $\overline{\rho} < 0$ and a left-hand screw for $\overline{\rho} < 0$. This velocity field has
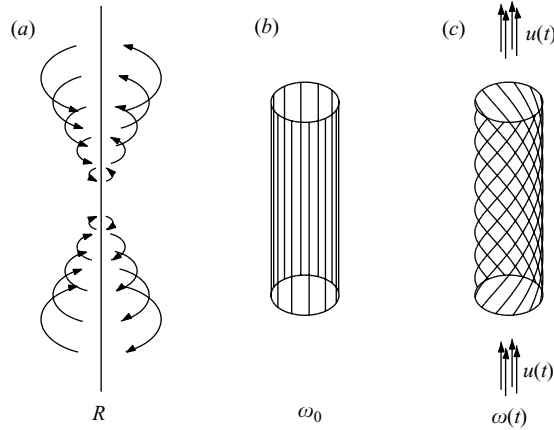
FIGURE 3. *Helicity cascade by vortex twisting*. (*b*) A cylindrical tube of parallel vortex lines in (*a*) a constant screw field with twisting direction along the vortex axis. (*c*) The result is that the vortex lines are twisted into helices. The tilting of the small scale vorticity vector and the solenoidal generation of an axial velocity create helicity at small scales. A positive (tensile) stress occurs, in the plane perpendicular to the vortex axis at loose winding and along the twist axis at tight winding.

both non-vanishing strain and vorticity:

$$\overline{\mathbf{S}} = \begin{bmatrix} 0 & 0 & -\overline{\rho}y/4 \\ 0 & 0 & \overline{\rho}x/4 \\ -\overline{\rho}y/4 & \overline{\rho}x/4 & 0 \end{bmatrix}, \quad \overline{\boldsymbol{\omega}} = \begin{bmatrix} -\overline{\rho}x/2 \\ -\overline{\rho}y/2 \\ \overline{\rho}z \end{bmatrix}. \tag{5.38}$$

Furthermore, the vorticity-gradient matrix is constant and symmetric:

$$\nabla\overline{\boldsymbol{\omega}} = \begin{bmatrix} -\overline{\rho}/2 & 0 & 0 \\ 0 & -\overline{\rho}/2 & 0 \\ 0 & 0 & \overline{\rho} \end{bmatrix} = \overline{\mathbf{R}}. \tag{5.39}$$

It is not hard to check that the small-scale velocity field defined previously becomes an exact time-dependent solution of the 'rapid-distortion equation' $(\partial_t + \boldsymbol{u} \cdot \nabla)\boldsymbol{\omega}^{[k]}(t) = (\boldsymbol{\omega}^{[k]}(t) \cdot \nabla)\boldsymbol{u} = 0$, with $\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}^{[k]}(t)$, if the parameter $p = \overline{\rho}t$. (This is no longer equivalent to the full three-dimensional Euler equation, since the large scales also have vorticity, neglected here.) The small scales begin as the undisturbed vortex tube of Example 1, whose filaments are then twisted into helices by the large-scale screw. The resulting vorticity field of coiled helices generates the axial velocity $w^{[k]}$ of (5.35) by solenoidal action, producing a net helicity in the small-scales (see figure 3).

Let us now consider the helicity transfer process, based upon our general formulae for the stress. We shall only consider the space region $r < R$, since the small-scale fields outside the tube are the same as for Example 1. Inside the small-scale vortex tube the velocity-gradient tensor is

$$\mathbf{D}^{[k]}(x, y) = \tfrac{1}{2}\omega^{[k]} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ -px & -py & 0 \end{bmatrix}. \tag{5.40}$$

Substituting into (5.1) gives the stress,

$$\boldsymbol{\tau}_*^{[k],(1)} = \tfrac{1}{12}\overline{C}^{[k]}\big|\omega^{[k]}\ell_k\big|^2 \begin{bmatrix} 1 & 0 & py \\ 0 & 1 & -px \\ py & -px & p^2 r^2 \end{bmatrix}, \tag{5.41}$$

to first order in gradients. Unlike Example 1, all three terms in the stress formula (5.4) (or (5.9)) are present, including that from 'skew-strain'. When p is small ($p\ell_k \ll 1$), then this is essentially the same result as in Example 1, but when p is large ($p\ell_k \gg 1$), the dominant stress is tensile along the screw axis. The resulting helicity flux has the form

$$\Lambda_*^{[k],(1)} = \tfrac{1}{6}\overline{C}^{[k]}\overline{\rho}\big|\omega^{[k]}\ell_k\big|^2[1 - p^2 r^2]. \tag{5.42}$$

When p is small, there is a net transfer of helicity to the small scales of the same sign as the large-scale screw. This arises from the weakly local transfer produced by the large-scale vorticity gradient acting against the contractile stress along the small-scale vortex. However, for large p, the sign of helicity flux reverses, as the more tightly wound vortex lines produce a net tensile stress along the screw axis by solenoidal action. The contributions to helicity flux of the separate $\boldsymbol{S}^{(n)}\boldsymbol{S}^{(n)}$, $[\boldsymbol{\Omega}^{(n)}, \boldsymbol{S}^{(n)}]$, and $-\boldsymbol{\Omega}^{(n)}\boldsymbol{\Omega}^{(n)}$ stress terms in (5.9) are

$$-\tfrac{1}{48}\overline{C}^{[k]}\overline{\rho}\big|p\omega^{[k]}\ell_k\big|^2 r^2, \quad -\tfrac{1}{8}\overline{C}^{[k]}\overline{\rho}\big|p\omega^{[k]}\ell_k\big|^2 r^2, \quad \tfrac{1}{6}\overline{C}^{[k]}\overline{\rho}\big|\omega^{[k]}\ell_k\big|^2\left[1 - \tfrac{1}{8}p^2 r^2\right], \tag{5.43}$$

respectively. We see that the flux comes mainly from the $-\boldsymbol{\Omega}^{(n)}\boldsymbol{\Omega}^{(n)}$ term for $p\ell_k \ll 1$, as claimed above. For $p\ell_k \gg 1$, all three terms contribute, with the flux contribution from the 'skew-strain' six times bigger than that of either of the other terms.

This example also illustrates the cascade of energy. Indeed, as was observed by Brissaud *et al.* (1973), the transfer of helicity necessarily involves also the transfer of energy. The formula (5.41) for the small-scale stress and (5.38) for the large-scale strain yield the following result for energy flux:

$$\Pi_*^{[k],(1)} = \tfrac{1}{24}\overline{C}^{[k]}\overline{\rho}p\big|\omega^{[k]}\ell_k\big|^2 r^2. \tag{5.44}$$

There is a net forward transfer of energy if the signs of $\overline{\rho}$ and p are the same. In that case, the large-scale screw winds the small-scale helical vortex lines more tightly, and kinetic energy is generated in the axial velocity component by the resulting solenoidal action. The contributions to energy flux of the separate $\boldsymbol{S}^{(n)}\boldsymbol{S}^{(n)}$, $[\boldsymbol{\Omega}^{(n)}, \boldsymbol{S}^{(n)}]$, and $-\boldsymbol{\Omega}^{(n)}\boldsymbol{\Omega}^{(n)}$ stress terms in (5.9) are

$$0, \quad \tfrac{1}{48}\overline{C}^{[k]}\overline{\rho}p\big|\omega^{[k]}\ell_k\big|^2 r^2, \quad \tfrac{1}{48}\overline{C}^{[k]}\overline{\rho}p\big|\omega^{[k]}\ell_k\big|^2 r^2, \tag{5.45}$$

respectively. Inside the vortex, there is no energy transfer from the strain-squared and, instead, equal amounts of the energy flux are due to the contractile stress along vortex lines and the stress proportional to 'skew-strain'.

6. Conclusions

In this paper we have developed a novel approximation for turbulent stress, via a multi-scale gradient (MSG) expansion. This scheme represents the stress by an expansion in scales of motion and in orders of space gradients. A major result (Appendix A) is that this expansion converges and furthermore at a rapid rate for the 'strongly local' part of the stress from the resolved scales and adjacent subscales. However, the convergence of the spatial Taylor expansion is expected

to be much slower for stress contributions from scales further below the filtering scale. Therefore, we have developed a more approximate expansion, which should give a reasonable result at all scales with just a few low-order velocity gradients. This 'coherent-subregions approximation' (CSA) is based on the assumption that the velocity increments across all the subscale separation vectors should give a similar result, at a given scale, as those for separation vectors in a 'shell' where the gradient expansion is accurate and rapidly convergent.

An important application of our methods has been presented to the three-dimensional turbulent cascades of energy and helicity. Our main results are the formulae (5.4) for the stress, (5.10) for the energy flux, and (5.25) for the helicity flux, exact to first-order in gradients. We have also developed the corresponding CSA expressions, (5.2), (5.13) and (5.26), which are more heuristic, but which should give a better representation of the very small-scale contributions than the exact first-order results. We have generalized Betchov's well-known relation, which relates mean vortex-stretching and strain-skewness at the same scale, to a similar relation between different scales ((5.12) and Appendix D). This relation allowed us to derive expression (5.14) for mean energy flux and (5.34) for mean helicity flux, and to analyse the expected contributions at different scales. Finally, we have discussed the physical mechanisms of energy and helicity cascade, in terms of our analytical formulae. We have shown by means of simple exact solutions of three-dimensional Euler equations that our results are consistent with energy transfer by Taylor's mechanism of 'vortex-stretching' and with helicity transfer by a mechanism of 'vortex-twisting'.

There are many implications of the present work for experiment and simulation, for theory, and for modelling.

A host of testable predictions have been provided for laboratory experiment and for numerical simulation by our detailed formulae for turbulent stress, energy flux and helicity flux. The expansions in scale and in space have been proved to converge, but the rate of convergence could be even faster than what has been rigorously established and empirical studies can determine this. The very distant subscales have been proved in Eyink (2005) to give decreasing contributions to stress, and analytical closures make further quantitative predictions about the mean amount of energy and helicity transfer from each scale of motion (e.g. see Kraichnan 1971; André & Lesieur 1977). Our multiscale formalism provides a convenient framework within which to check these predictions, particularly for experimentalists who cannot easily calculate spectral transfers. As to the gradient expansion, our first-order expressions (5.4), (5.10) and (5.25) should give good results for the strongly local contributions, without further approximations. Experiment and simulation can also check the validity of our CSA expansion, which is based upon a bolder assumption. Assuming that our results are empirically confirmed, experiment and simulation can also determine the relative magnitudes of the various terms in our formulae. This will help to shed further light on the detailed physical mechanisms which underlie the turbulent cascades.

Our results suggest several further fruitful directions for theory. Previous dynamical models of velocity gradients (Vieillefosse 1982, 1984; Cantwell 1992; Chertkov *et al.* 1999) have investigated only alignments between objects at the same scale. However, as our results should make evident, alignments between velocity gradients at distinct scales are also of great importance in supporting turbulent cascades and these inter-scale relations have received scant attention so far. Improvement of our various approximations is another important avenue for theory, particularly the CSA scheme, where many possible refinements are apparent. Finally, theoretical methods to estimate subscale velocity gradients from the resolved ones are strongly motivated

by our work. This would lead to LES modelling schemes, similar to those reviewed in Domaradzki & Adams (2002), but based upon a clearer picture of the physical processes involved. If there is a universal mechanism which generates small scales from large scales, then modelling this generation process should lead to the most robust and generally applicable LES models.

A virtue of our approach is its wide range of potential applications. Since it is based upon a very general feature of turbulent cascades – i.e. their locality in scale and in space – the same scheme of approximation can be exploited in many different situations, with, of course, differing results depending upon the particular circumstances. For example, in Eyink (2006), we apply our methods to the cascade of energy in two-dimensions and obtain results consistent with an inverse cascade. In this case, it is a weakly local interaction via the 'skew-strain' which plays the fundamental dynamical role. We anticipate many other useful applications, such as passive scalar cascades and magnetohydrodynamic cascades of energy and magnetic helicity. We hope that our method will be useful for all these cases in illuminating the physical mechanisms involved.

Appendix A. Convergence of the gradient expansion

We establish here the convergence of the stress approximation $\tau^{(n,m)}$ in the limit $m \to \infty$, for the space L^1-norm. The advantage of this norm is that it allows us to give the proof by entirely elementary methods (although convergence can doubtless be established also using other L^p norms for $p > 1$). We also give the proof, again for simplicity, in infinite volume in d-dimensions without flow boundaries.

Our argument uses the formula

$$\tau^{(n,m)} = \int d^d r \, G_\ell(r) \delta u^{(n,m)}(r) \delta u^{(n,m)}(r) - \int d^d r \, G_\ell(r) \delta u^{(n,m)}(r) \int d^d r \, G_\ell(r) \delta u^{(n,m)}(r),$$
(A 1)

with

$$\delta u^{(n,m)}(r; x) = \sum_{p=1}^{m} \frac{1}{p!} (r \cdot \nabla)^p u^{(n)}(x).$$
(A 2)

If Γ has a compactly supported Fourier transform, then $u^{(n)}(x)$ is real-analytic and thus $\delta u^{(n,m)}(r; x) \to \delta u^{(n)}(r; x)$ as $m \to \infty$, pointwise in x and also, as we see below, in the L^1 norm. Therefore, it is enough to establish absolute integrability and summability:

$$\int d^d r \, G_\ell(r) \sum_{p,p'=0}^{\infty} \frac{1}{p! p'!} \left\| (r \cdot \nabla)^p u^{(n)} (r \cdot \nabla)^{p'} u^{(n)} \right\|_1 < \infty$$
(A 3)

and

$$\int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r}) \int \mathrm{d}^d\boldsymbol{r}'\, G_\ell(\boldsymbol{r}') \sum_{p,p'=0}^{\infty} \frac{1}{p!p'!} \left\|(\boldsymbol{r}\cdot\boldsymbol{\nabla})^p\boldsymbol{u}^{(n)}(\boldsymbol{r}'\cdot\boldsymbol{\nabla})^{p'}\boldsymbol{u}^{(n)}\right\|_1 < \infty. \tag{A 4}$$

In that case, the integrations and infinite summations commute and

$$\lim_{m\to\infty} \boldsymbol{\tau}^{(n,m)} = \int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r})\delta\boldsymbol{u}^{(n)}(\boldsymbol{r})\delta\boldsymbol{u}^{(n)}(\boldsymbol{r}) - \int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r})\delta\boldsymbol{u}^{(n)}(\boldsymbol{r}) \int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r})\delta\boldsymbol{u}^{(n)}(\boldsymbol{r})$$
$$= \boldsymbol{\tau}^{(n)}. \tag{A 5}$$

Let us establish the bound (A 3). By the Cauchy–Schwartz inequality,

$$\left\|(\boldsymbol{r}\cdot\boldsymbol{\nabla})^p\boldsymbol{u}^{(n)}(\boldsymbol{r}\cdot\boldsymbol{\nabla})^{p'}\boldsymbol{u}^{(n)}\right\|_1 \leqslant |\boldsymbol{r}|^{p+p'}\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2\left\|\boldsymbol{\nabla}^{p'}\boldsymbol{u}^{(n)}\right\|_2. \tag{A 6}$$

Thus, (A 3) is implied by

$$\int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r}) \left[\sum_{p=0}^{\infty} \frac{1}{p!}|\boldsymbol{r}|^p\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2\right]^2 < \infty. \tag{A 7}$$

By a similar argument, we see that (A 4) holds, if

$$\int \mathrm{d}^d\boldsymbol{r}\, G_\ell(\boldsymbol{r}) \left[\sum_{p=0}^{\infty} \frac{1}{p!}|\boldsymbol{r}|^p\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2\right] < \infty. \tag{A 8}$$

To proceed we must have an estimate of $\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\|_2$. This is easy to obtain by going over to Fourier transforms using the Plancherel identity:

$$\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2^2 = \int \mathrm{d}^d\boldsymbol{k}\left|(\mathrm{i}\boldsymbol{k})^p\,\widehat{\Gamma}(\ell_n\boldsymbol{k})\,\widehat{\boldsymbol{u}}(\boldsymbol{k})\right|^2. \tag{A 9}$$

Since $\widehat{\Gamma}$ has compact support, the integral over $\boldsymbol{k}$ involves only the wavenumbers with $|\boldsymbol{k}| < c_1/\ell_n$ for some constant c_1. Thus,

$$\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2^2 \leqslant c_2^2(c_1/\ell_n)^{2p} \int \mathrm{d}^d\boldsymbol{k}\,|\widehat{\boldsymbol{u}}(\boldsymbol{k})|^2, \tag{A 10}$$

for another constant $c_2 = \sup_{\boldsymbol{k}}|\widehat{\Gamma}(\boldsymbol{k})|$, or

$$\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2 \leqslant c_2(c_1/\ell_n)^p\|\boldsymbol{u}\|_2. \tag{A 11}$$

With this estimate we obtain

$$\sum_{p=0}^{\infty} \frac{1}{p!}|\boldsymbol{r}|^p\left\|\boldsymbol{\nabla}^p\boldsymbol{u}^{(n)}\right\|_2 \leqslant c_2\exp(c_1|\boldsymbol{r}|/\ell_n)\|\boldsymbol{u}\|_2. \tag{A 12}$$

Thus, we see that (A 7) and (A 8) hold, if the filter kernel $G(\boldsymbol{r})$ decays faster than exponentially in space. For example, G could be Gaussian. Notice that $\Gamma(\boldsymbol{r})$ can also decay very rapidly in space – for example, faster than any inverse power – since the Fourier transform $\widehat{\Gamma}(\boldsymbol{k})$ may be both compactly supported and C^∞. For any such filter kernels G and Γ, we conclude finally that the absolute summability/integrability conditions (A 3),(A 4) both hold, and thus the limit relation (A 5) is valid, as claimed. QED.

Appendix B. Comparison with the defiltering approach

As mentioned in §1, Yeo & Bedford (1988), Leonard (1997), and Carati *et al.* (2001) have developed a somewhat similar gradient expansion for the turbulent stress. Here we would like to compare and contrast the two approaches and, in particular, indicate our reasons for dissatisfaction with the expansion constructed by those authors. Their approach is based upon *defiltering*, which is the inverse to the filtering operator, defined spectrally by

$$\mathscr{G}_\ell \boldsymbol{v}(\boldsymbol{x}) = \int \mathrm{d}^d \boldsymbol{k} \; \widehat{G}(\boldsymbol{k}\ell)\widehat{\boldsymbol{v}}(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{B 1}$$

Thus, the defiltering operator is given similarly by

$$\mathscr{G}_\ell^{-1} \boldsymbol{v}(\boldsymbol{x}) = \int \mathrm{d}^d \boldsymbol{k} \; [\widehat{G}(\boldsymbol{k}\ell)]^{-1}\widehat{\boldsymbol{v}}(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{B 2}$$

In terms of these operators, Yeo & Bedford (1988); Leonard (1997) and Carati *et al.* (2001) define a tensor-valued functional

$$T[\boldsymbol{v}] \equiv \mathscr{G}_\ell\{\mathscr{G}_\ell^{-1}\boldsymbol{v} \; \mathscr{G}_\ell^{-1}\boldsymbol{v}\} - \boldsymbol{v} \; \boldsymbol{v}. \tag{B 3}$$

A little thought shows that if $\overline{\boldsymbol{u}} = \mathscr{G}_\ell \boldsymbol{u}$ is substituted into this functional, then we recover the turbulent stress as $\boldsymbol{\tau} = T[\overline{\boldsymbol{u}}]$. Hence, this formula provides, seemingly, an exact closure of the stress in terms of the filtered velocity $\overline{\boldsymbol{u}}$. Furthermore, the functional T has a formal gradient expansion:

$$T_{ij}[\boldsymbol{v}] = \sum_{\boldsymbol{p},\boldsymbol{q}} c_{\boldsymbol{p},\boldsymbol{q}} \nabla^{\boldsymbol{p}} v_i \; \nabla^{\boldsymbol{q}} v_j, \tag{B 4}$$

where the summation is over multi-indices $\boldsymbol{p} = (p_1, \ldots, p_d)$, $\boldsymbol{q} = (q_1, \ldots, q_d)$ with integer components. Note that $\nabla^{\boldsymbol{p}} = \partial_1^{p_1} \cdots \partial_d^{p_d}$ for the multi-index $\boldsymbol{p}$. The coefficients in the expansion (B 4) can be obtained from a generating function (Carati *et al.* 2001):

$$F[\boldsymbol{\phi}, \boldsymbol{\psi}] \equiv \frac{\widehat{G}(-\mathrm{i}(\boldsymbol{\phi} + \boldsymbol{\psi}))}{\widehat{G}(-\mathrm{i}\boldsymbol{\phi})\widehat{G}(-\mathrm{i}\boldsymbol{\psi})} = \sum_{\boldsymbol{p},\boldsymbol{q}} c_{\boldsymbol{p},\boldsymbol{q}} \boldsymbol{\phi}^{\boldsymbol{p}} \boldsymbol{\psi}^{\boldsymbol{q}}.$$

Here $\boldsymbol{\phi}^{\boldsymbol{p}} = \phi_1^{p_1} \cdots \phi_d^{p_d}$. Thus, the expansion (B 4) for $\boldsymbol{\tau} = T[\overline{\boldsymbol{u}}]$ seems to yield a closed constitutive formula for the turbulent stress in terms of the gradients of the filtered velocity.

To see the problem with this approach, note that the defiltering operator is not even defined if the filter kernel has a compactly supported Fourier transform. In this case, all the subscale modes cannot be recovered from knowledge of the filtered velocity $\overline{\boldsymbol{u}}$. However, this is only an extreme form of a general difficulty. For any filter kernel G, the defiltering operator $\mathscr{G}_\ell^{-1}$ is unbounded on the natural function spaces for the velocity field, such as the L^p spaces. This means that defiltering is not defined for every element of those spaces, but instead only for a (dense) subspace, called the 'domain' of the operator. The natural, maximal domain of the defiltering operator in any of these spaces is the range of the corresponding filtering operator on that space, or $\mathrm{Dom}(\mathscr{G}_\ell^{-1}) = \mathrm{Ran}(\mathscr{G}_\ell)$. This means that, to defilter a function in the space, that element must have been obtained by filtering another member of the space. However, this is not the case for most functions in the space, even infinitely smooth ones.

For example, consider the most natural space of L^2 or finite-energy fields, and a Gaussian filter kernel G. Most $\boldsymbol{v} \in L^2$, even those with very rapidly decaying Fourier

coefficients $\widehat{\boldsymbol{v}}(\boldsymbol{k})$, have no Gaussian defilter. Formally,

$$\left[\mathscr{G}_\ell^{-1}\boldsymbol{v}\right]^\smallfrown(\boldsymbol{k}) = \exp[+(k\ell)^2/2\sigma^2]\widehat{\boldsymbol{v}}(\boldsymbol{k}) \qquad (\text{B}\,5)$$

for a Gaussian kernel with Fourier transform $\widehat{G}(\boldsymbol{k}) = \exp(-k^2/2\sigma^2)$. Thus, the Fourier coefficients $\widehat{\boldsymbol{v}}(\boldsymbol{k})$ might decay very rapidly, e.g. exponentially in $|\boldsymbol{k}|$, and yet the defiltered field has infinite energy or $\mathscr{G}_\ell^{-1}\boldsymbol{v} \notin L^2$. For such a velocity field, the stress $\boldsymbol{T}[\boldsymbol{v}]$ defined by (B 3) does not exist. This poses a real difficulty for an LES closure equation based upon a constitutive relation $\boldsymbol{\tau} = \boldsymbol{T}^{(m)}[\overline{\boldsymbol{u}}]$ obtained by truncating the expansion (B 4) at finite order m. There is nothing to guarantee that the solution $\overline{\boldsymbol{u}}$ of such a closure equation will have Fourier coefficients decaying fast enough for (B 5) to remain in L^2. In that case, the expansion (B 4) will not converge and there is no reason to expect that the solution of the mth-order LES equation will converge in the limit $m \to \infty$ to the exact filtered velocity, even though the closure then becomes formally 'exact'. Of course, even worse, the LES equation may itself be ill-posed and its solution could blow up at finite time. The 'exactness' of the closure as $m \to \infty$ does not provide any guarantee of good behaviour at finite m.

Such difficulties with defiltering are not unknown in the LES literature. Domaradzki & Adams (2002) have reviewed various approaches to subgrid stress modelling by defiltering and have pointed out the related fact that defiltering is generally an ill-posed operation in function space. In particular, multiplication by the inverse filter transform, as in our equation (B 5), magnifies the effects of noise and round-off error at high wavenumbers. Thus, the defiltering operation, even when it exists, is not stable to small perturbations in the input velocity field. As in any ill-posed problem, various regularizations may be considered to render it well-posed. Most of the existing approaches have employed an approximate regularized defiltering together with an 'eddy-viscosity' or dissipative term at high wavenumbers (see Domaradzki & Adams 2002). Needless to say, our approach is quite different. We have constructed an approximation scheme which is proved to converge under very modest assumptions, but which is not closed. Our present goal is to develop a tool to explore the basic physics and not to construct turbulence models directly. Our expressions for turbulent stress may be useful in modelling efforts, but we must defer to future work the important problem of estimating the unknown subscale gradients that appear.

Appendix C. CSA expansion coefficients for Gaussian kernel

We give here the coefficients that appear in the CSA expansion, for the special case of an isotropic Gaussian filter:

$$G_\ell(\boldsymbol{r}) = \frac{1}{[2\pi(\sigma\ell)^2]^{d/2}} \exp\left[-\frac{r^2}{2(\sigma\ell)^2}\right].$$

In general, one would like to have $\sigma \approx 1$, so that this really corresponds to a filter at scale ℓ. However, this is often not true; for example, the conventional choice made by Leonard (1974) was $\sigma^2 = 1/12$ (so that the second moment of the Gaussian and box filters would agree). In such cases, it is better to define the 'shells' in the model formulation as

$$\mathscr{S}_0 = \{\boldsymbol{r} : |\boldsymbol{r}| > \sigma\ell_0\}, \qquad (\text{C}\,1)$$

$$\mathscr{S}_k = \{\boldsymbol{r} : \sigma\ell_{k-1} > |\boldsymbol{r}| > \sigma\ell_k\}, \quad k = 1, \ldots, n. \qquad (\text{C}\,2)$$

In this way, increments for separations $r \approx \sigma \ell_n$ are calculated from fields $\boldsymbol{u}^{(n)}$ filtered at the same length scale. We must calculate the partial averages of $|\boldsymbol{r}|^p$, $p = 2, 4, 6 \ldots$ with respect to the Gaussian filter, over each of these shells. Introducing a dimensionless variable $\boldsymbol{\rho} = \boldsymbol{r}/\ell$, these moment averages may be written as $C_p^{[k]} \ell^p$ for shell $\mathscr{S}_k$, $k = 0, 1, \ldots, n$.

The integrals for coefficients $C_p^{[k]}$ are evaluated by substituting $t = \rho^2/(2\sigma^2)$, $\sigma^2 \mathrm{d}t = \rho \mathrm{d}\rho$, and using $S_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$ for the $(d-1)$-volume of the unit sphere in dimension d:

$$
\begin{aligned}
C_p^{[0]} &= S_{d-1} \int_\sigma^\infty \rho^{d+p-1} \frac{\mathrm{e}^{-\rho^2/2\sigma^2}}{(2\pi\sigma^2)^{d/2}} \, \mathrm{d}\rho \\
&= \frac{(2\sigma^2)^{p/2}}{\Gamma(d/2)} \int_{1/2}^\infty t^{(d+p)/2-1} \mathrm{e}^{-t} \, \mathrm{d}t = \frac{2^{p/2}}{\Gamma(d/2)} \Gamma\left(\frac{d+p}{2}, \frac{1}{2}\right) \sigma^p,
\end{aligned} \tag{C 3}
$$

and

$$
\begin{aligned}
C_p^{[k]} &= S_{d-1} \int_{\sigma\lambda^{-k}}^{\sigma\lambda^{-(k-1)}} \rho^{d+p-1} \frac{\mathrm{e}^{-\rho^2/2\sigma^2}}{(2\pi\sigma^2)^{d/2}} \, \mathrm{d}\rho \\
&= \frac{2^{p/2}}{\Gamma(d/2)} \left[\gamma\left(\frac{d+p}{2}, \frac{1}{2\lambda^{2(k-1)}}\right) - \gamma\left(\frac{d+p}{2}, \frac{1}{2\lambda^{2k}}\right)\right] \sigma^p,
\end{aligned} \tag{C 4}
$$

for $k = 1, \ldots, n$. Here, we have introduced the incomplete gamma functions $\Gamma(a, x)$ and $\gamma(a, x) = \Gamma(a) - \Gamma(a, x)$, as they are defined in the standard literature (Abramowitz & Stegun 1964).

The asymptotics of these coefficients for large k are obtained using $\gamma(a, x) \sim x^a/a$ as $x \to 0$ (e.g. Abramowitz & Stegun 1964, 6.5.4 and 6.5.29). Thus,

$$
C_p^{[k]} \sim C(d, p, \lambda) \lambda^{-(d+p)k} \sigma^p, \quad k \to \infty,
$$

with $C(d, p, \lambda) = (\lambda^{d+p} - 1)/[(d + p)\Gamma(d/2)2^{(d-2)/2}]$. If we define $\overline{C}_p^{[k]} = \lambda^{(d+p)k} C_p^{[k]}$, then this new constant becomes independent of k as $k \to \infty$:

$$
\overline{C}_p^{[k]} \sim C(d, p, \lambda) \sigma^p. \tag{C 5}
$$

It is not hard to prove that these same asymptotics hold, at least as big-O bounds, for much more general filter kernels than Gaussian.

An interesting application of (C 5) is to establish the order of magnitude of the 'systematic' stress term $\boldsymbol{\varrho}_*^{[k],(m)}$ that appears in equation (4.13) for $\boldsymbol{\tau}_*^{[k],(m)}$. We assume that the velocity field $\boldsymbol{u}$ has the Hölder exponent $0 < \alpha < 1$. From the definition (4.10), it is obvious that $\boldsymbol{\varrho}_*^{[k],(m)}$ is a sum over $p, p' = 0, \ldots, m$ of terms proportional to

$$
\overline{C}_{p+p'}^{[k]} \ell_k^{p+p'} \left(\partial^p \boldsymbol{u}^{[k]}\right)\left(\partial^{p'} \boldsymbol{u}^{[k]}\right). \tag{C 6}
$$

Here, $\partial^p \boldsymbol{u}^{[k]}$ indicates a pth-order space derivative of $\boldsymbol{u}^{[k]}$ with component indices suppressed. It is not hard to show (e.g. see Eyink 2005) that $\partial^p \boldsymbol{u}^{[k]} = O(\ell_k^{\alpha-p})$. On the other hand, (C 5) implies that $\overline{C}_{p+p'}^{[k]}$ is asymptotically constant as $k \to \infty$. It follows that each term p, p' of the Taylor expansion contributes a term for $\boldsymbol{\varrho}_*^{[k],(m)}$ that scales as $O(\ell_k^{2\alpha})$. In fact, this is the correct order of magnitude for the contribution to the stress from length scale ℓ_k (Eyink 2005). It is worth pointing out that the term $\boldsymbol{u}_*'^{[k],(m)} \boldsymbol{u}_*'^{[k'],(m)}$ in (4.13) would likewise scale as $O(\ell_k^\alpha \ell_{k'}^\alpha)$, if the correction factor N_k had been used in the definition (4.12) rather than $N_k^{1/2}$. Indeed, so defined, $\boldsymbol{u}_*'^{[k],(m)} \boldsymbol{u}_*'^{[k'],(m)}$ is from (4.10) a sum over p, p' of terms proportional to $\overline{C}_p^{[k]} \overline{C}_{p'}^{[k']} \ell_k^p \ell_{k'}^{p'} (\partial^p \boldsymbol{u}^{[k]})(\partial^{p'} \boldsymbol{u}^{[k']})$.

In that case, the previous argument carries through. It might seem that this alternative definition of $u_*'^{[k],(m)}$ therefore has some merit, except that it ignores the cancellations that we expect to occur in the integrals over volume.

Appendix D. Generalized Betchov relation in three dimensions

We here give briefly the proof of the generalized Betchov relation (5.12). Let us suppose that a, b, c are three solenoidal (divergence-free) vector fields in three dimensions. Then, it is trivial to verify from the product rule of differentiation that

$$a_{i,j}b_{j,k}c_{k,i} + c_{k,j}b_{j,i}a_{i,k} = \partial_i(a_{i,j}b_{j,k}c_k) - \partial_k(a_{i,j}b_{j,i}c_k) + \partial_j(a_{i,k}b_{j,i}c_k), \tag{D 1}$$

where we use the notation $a_{i,j} = \partial a_i / \partial x_j$, etc. Because the right-hand side is a total space derivative, the ensemble average of the left-hand side is zero if we assume space homogeneity:

$$\langle a_{i,j}b_{j,k}c_{k,i} + c_{k,j}b_{j,i}a_{i,k} \rangle = 0. \tag{D 2}$$

This same relation holds for space averages, if boundary conditions on a, b, c are such that boundary terms from integration by parts can be ignored. With either of these assumptions, let us then apply (D 2) for $b = \overline{u}$ and $a = c = u^{(n)}$. This gives

$$\left\langle \mathrm{Tr}\left[\overline{\boldsymbol{D}}(\boldsymbol{D}^{(n)})^2\right] \right\rangle = 0, \tag{D 3}$$

with $D_{ij} = u_{i,j}$ the deformation matrix associated to a velocity field $\boldsymbol{u}$.

Now, using $D_{ij}^{(n)} = S_{ij}^{(n)} - (1/2)\epsilon_{ijk}\omega^{(n)}$ (equation (5.3)) gives

$$\begin{aligned} \left(\boldsymbol{D}^{(n)}\right)^2 = \left(\boldsymbol{S}^{(n)}\right)^2 &- \tfrac{1}{4}\left(\boldsymbol{I}\big|\boldsymbol{\omega}^{(n)}\big|^2 - \boldsymbol{\omega}^{(n)}\boldsymbol{\omega}^{(n)}\right) \\ &+ \tfrac{1}{2}\left(\boldsymbol{\omega}^{(n)} \times \boldsymbol{S}^{(n)} + \boldsymbol{S}^{(n)} \times \boldsymbol{\omega}^{(n)}\right). \end{aligned} \tag{D 4}$$

Note that the matrices on the first line of the right-hand side are symmetric and the matrix on the second line is antisymmetric. ($\boldsymbol{I}$ is the identity matrix.) Thus, if we use the relation analogous to (5.3) for $\overline{D}_{ij}$, then the only contribution to the trace of $\overline{\boldsymbol{D}}$ with $(\boldsymbol{D}^{(n)})^2$ is from the trace of $\overline{S}_{ij}$ with the first line in (D 4) and from the trace of $\epsilon_{ijk}\overline{\omega}_k/2$ with the second line. Using tracelessness of the strain matrix $\overline{\boldsymbol{S}}$ and the identity $\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$ gives

$$\mathrm{Tr}\left[\overline{\boldsymbol{D}}(\boldsymbol{D}^{(n)})^2\right] = \mathrm{Tr}\left(\overline{\boldsymbol{S}}(\boldsymbol{S}^{(n)})^2\right) + \tfrac{1}{4}\left(\boldsymbol{\omega}^{(n)}\right)^\top \overline{\boldsymbol{S}}\left(\boldsymbol{\omega}^{(n)}\right) + \tfrac{1}{2}(\overline{\boldsymbol{\omega}})^\top \boldsymbol{S}^{(n)}\left(\boldsymbol{\omega}^{(n)}\right). \tag{D 5}$$

Substituting (D 5) into (D 3) gives (5.12). QED.

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