Stochastic self-energy subgrid model for the large eddy simulation of turbulent channel flows

V Kitsios¹,², JA Sillero³, J Soria¹,⁴ and JS Frederiksen²

¹ Laboratory For Turbulence Research in Aerospace and Combustion, Department of Mechanical and Aerospace Engineering, Monash University, Clayton 3800, AUSTRALIA
² Centre for Australian Weather and Climate Research, CSIRO Marine and Atmospheric Research, 107-121 Station St, Aspendale 3195, AUSTRALIA
³ School of Aeronautics, Universidad Politécnica de Madrid, Pza. Cardenal Cisneros 3, E-28040 Madrid, SPAIN
⁴ Department of Aeronautical Engineering, King Abdulaziz University, Jeddah, KINGDOM OF SAUDI ARABIA.

E-mail: vassili.kitsios@monash.edu, sillero@torroja.dmt.upm.es, julio.soria@monash.edu, jorgen.frederiksen@csiro.au

Abstract. This paper presents the large eddy simulation (LES) of turbulent channel flow using a self-energy (SE) subgrid model with coefficients determined from reference direct numerical simulations (DNSs). In contrast to standard approaches that develop subgrid models based upon physical hypotheses, in the present SE approach the model coefficients are determined from the subgrid statistics of a DNS, with physical interpretations made post hoc. This technique is applied here for the first time to wall-bounded flows, specifically channel flow. The stochastic SE subgrid model consists of a mean field shift, deterministic drain dissipation acting on the resolved field and a stochastic backscatter force. The deterministic SE subgrid model comprises of a net dissipation representing the net effect of the drain and backscatter. We present LESs that reproduce the time-averaged kinetic energy spectra of the DNS within the resolved scales. The direction and magnitude of the energy transfers in scale space can then be determined from the coefficients of the SE subgrid model. Results are presented for friction velocity based Reynolds numbers up to \(Re_\tau = 950\).

1. Introduction

With the current level of algorithmic and computational hardware technology, it is not possible to simulate industrial nor geophysical flows at typical Reynolds numbers of interest by explicitly resolving all scales of motion. Instead one resorts to large eddy simulation (LES), where the large eddies are explicitly resolved on a computational grid and the unresolved subgrid-scale interactions are parameterised (or modelled). There have been many approaches taken to parameterise the subgrid interactions. The empirical Smagorinsky subgrid model [1] is one of the most widely adopted and celebrated. In this model the subgrid interactions are represented by an eddy viscosity determined from the product of the resolved strain rate, the local grid spacing and a specified tuning parameter. The next major development in this area was the Dynamic Smagorinsky model [2, 3], where the eddy viscosity was calculated from the scales resolved in a test filter at each step, and again assuming a similar relationship between the subgrid stresses and the resolved strain rate. In other physically justified approaches subgrid
models have been developed that are representative of idealised vortex structures observed in isotropic homogeneous turbulence and wall-bounded flows [4, 5]. Regardless of the approach, if the subgrid interactions are not self-consistently represented then an increase in resolution will not necessarily increase the accuracy of the explicitly resolved scales.

As in general it is only possible to parameterise the statistical effects of the subgrid eddies [6], statistical dynamical closure theory is the natural formulation for developing self-consistent subgrid models. In closure calculations, equations are solved for the time varying statistical moments of the flow, as opposed to the instantaneous fields. The pioneering study in this area was the parameter-free Eulerian direct interaction approximation (DIA), developed for isotropic homogeneous turbulence [7]. In this closure the tendency of the transient component consists of a nonlinear damping and a nonlinear noise term. The self-consistent field theory [8] and the local energy transfer theory [9, 10] were developed independently, and shown to differ from the DIA only in the implementation of the fluctuation dissipation theorem [11, 12, 13]. Later a general theory of eddy viscosity for two- and three-dimensional homogeneous turbulence was developed in [14], which identified that in spectral space the eddy viscosity has a strong cusp-like form increasing with wavenumber up until the smallest resolved scale of motion. Additional statistical dynamical closure studies pertaining mainly to three-dimensional homogeneous turbulence include [15, 16, 17, 18, 19, 6, 20].

In the vast majority of studies, and in all of the aforementioned ones other than the DIA of [7], a physical hypothesis is proposed from which a subgrid model is developed. In contrast the following closure studies have made no assumptions on the physical relationship between the resolved and subgrid scales, with the model coefficients determined from higher resolution simulations. For homogeneous barotropic (two-dimensional) flow on a sphere, a self-consistent stochastic subgrid parameterisation was developed based on the DIA closure in [21], which comprised of a drain eddy viscosity and stochastic backscatter force. Backscatter is the physical process by which kinetic energy is transferred from small to large scales. A deterministic variant was also developed comprising of a net eddy viscosity representing the net effect of the drain and backscatter. These subgrid coefficients were determined from higher resolution closure calculations, and produced LESs that replicated the kinetic energy spectra of the benchmark simulation. For inhomogeneous turbulent flows, general expressions were later derived for the eddy viscosities, stochastic backscatter, meanfield shift, and eddy-topographic force based on a quasi-diagonal DIA (QDIA) closure in [22]. The various subgrid terms for atmospheric flows using the QDIA formalism were then evaluated in [23]. Each of the coefficients relating the subgrid tendency to the associated resolved quantities (mean field, fluctuating field or roughness elements) are referred to in [24] by the term self-energy (SE). More generally a self-energy is a linear operator that closes the effect of unresolved nonlinear processes on the resolved field [25, 26].

To broaden the applicability of the closure methods discussed above, a stochastic modelling approach was developed in [27] that determines the subgrid coefficients from the statistics of a higher resolution reference simulation solving for the instantaneous flow fields. The reference simulation is truncated back to a coarser grid and the eddy viscosities are then determined from the subgrid statistics, in a similar vein to the self-consistent closure calculations discussed above. We refer to this technique as the SE subgrid modelling approach, as it is essentially a numerical means of determining the SE closure coefficients. This approach has been successfully applied to quasi-geostrophic (QG) simulations of the atmosphere and ocean, comprising of sheared jets, Rossby waves, and baroclinic instability [28, 29, 30]. In addition, if the resolution of the LES is such that the smallest scales lie within a self-similar inertial range, then the subgrid coefficients may be governed by simple functions of resolution [31]. Using this approach eddy viscosity scaling laws have been developed for global QG simulations of the atmosphere [31] and ocean [32]. These scaling laws enable the subgrid parameterisations to be utilised more widely as they
remove the need to generate the subgrid coefficients from a reference simulation for these flows.

Recently, a unifying SE closure theory for the subgrid modelling of two- and three-dimensional inhomogeneous flows was developed in [33, 24]. The fundamental functional forms were determined for the four main types of subgrid interactions: eddy-eddy; eddy-meanfield; eddy-topographic; and meanfield-meanfield. Subgrid parametrisations representing these different interactions are calculated in [23]. Eddy-eddy interactions represent the impact unresolved subgrid eddies have on the evolution of the resolved eddies. The eddy-meanfield interactions represent the impact unresolved subgrid eddies have on the evolution of the resolved meanfield. The eddy-topographic (or eddy-roughness) form represents the interactions between the subgrid eddies and the resolved topography (or equivalently surface roughness). The meanfield-meanfield type represent the interactions between the unresolved subgrid meanfield and the resolved meanfield.

In the current study we use the SE subgrid modelling approach of [27] to systematically determine the model coefficients governing the subgrid interactions in simulations of horizontally periodic turbulent channel flows with smooth walls. Truncations are made at resolutions applicable to research-focused LES. This approach requires a direct numerical simulation (DNS) to determine the subgrid coefficients and is initially computationally expensive. However, not only does it produce LESs in very good agreement with the high resolution DNS, but also illuminates the true relationship between the resolved and subgrid scales and the energy transfers between them. As the present channel flow has smooth walls there is no eddy-topographic force. Additionally only the mode with both a spanwise and streamwise wavenumber of zero has non-zero mean under sufficient sampling, which means there is no subgrid meanfield and hence no meanfield-meanfield interactions. This type of interaction can be important, however, for flow configurations with complicated geometry and topography, as is the case of the ocean. The eddy-meanfield interactions are non-zero, but negligible in comparison to the dominant eddy-eddy interactions, which will be the focus of the present study. In section 2 we present the details of the DNS Navier-Stokes solver used in the turbulent channel flow simulations, and also characterise the base flow. The details on how the subgrid parameterisation coefficients are determined from the DNS statistics are then presented in section 3. The subgrid model coefficients are illustrated in section 4 decomposed in three-dimensional scale space, and by horizontal scale and vertical position in section 5. The ability of the LES to replicate the statistics of the DNS is then illustrated in section 6. Concluding remarks are made in section 7.

2. Direct Numerical Simulation
In the present study we solve the incompressible isothermal Navier-Stokes equations. In physical space the momentum and continuity equations are given by

\[
\frac{\partial u^a}{\partial t} + u^b \frac{\partial u^a}{\partial x^b} + \frac{1}{\rho} \frac{\partial p}{\partial x^a} - \nu \frac{\partial^2 u^a}{\partial x^a \partial x^b} = f_0^a, \quad \text{and} \quad \frac{\partial u^a}{\partial x^a} = 0, \tag{1}
\]

respectively, with the indices \(a = 1, 2, 3\) and \(b = 1, 2, 3\). The coordinates \((x^1, x^2, x^3) \equiv (x, y, z)\), where \(x\) is the streamwise direction, \(y\) the wall-normal, and \(z\) the spanwise. Likewise the velocity vector \((u^1, u^2, u^3) \equiv (u, v, w)\), where \(u\) is the streamwise direction, \(v\) the wall-normal, and \(w\) the spanwise velocity component. The force \(f_0^a\) symbolically represents the boundary conditions, \(\nu\) is the kinematic viscosity, and \(\rho\) the fluid density. The general spectral form of the equations is given by

\[
\frac{\partial}{\partial t} u^a_k(t) + D_{0b}^{ab}(k)u^b_k(t) = \sum_{k'} \sum_{k''} K^{abc}(k, k', k'')u^b_{-k'}(t)u^c_{-k''}(t) + f_0^a(k, t), \tag{3}
\]
Table 1. Numerical details of the channel simulations: friction-based Reynolds number ($Re_\tau \equiv u_\tau h/\nu$); centreline Reynolds number ($Re_0 \equiv u_0 h/\nu$); DNS truncation wavenumber ($T$); number of Chebyshev polynomials ($N$); domain sizes in streamwise, wall-normal and spanwise directions ($L_x$, $L_y$, $L_z$); in viscous units, the constant grid spacing in streamwise and spanwise directions ($\Delta x^+$, $\Delta z^+$) and the surface-normal grid spacing at the channel centreline ($\Delta y_{cl}^+$) and at the wall ($\Delta y_{wall}^+$); constant time-step size in viscous units ($\Delta t^+$); number of eddy turnover times over which the subgrid statistics were accumulated ($\langle t_f - t_i \rangle u_0/L_z$); LES truncation levels ($T_R$).

| $Re_\tau$ | $Re_0$ | $T$ | $N$ | ($L_x$, $L_y$, $L_z$) | ($\Delta x^+$, $\Delta y_{cl}^+$, $\Delta y_{wall}^+$, $\Delta z^+$) | $\Delta t^+$ | $\langle t_f - t_i \rangle u_0/L_z$ | $T_R$ |
|------------|--------|-----|-----|---------------------|---------------------------------|-------------|--------------------------|------|
| 180        | 3250   | 64  | 97  | (2$\pi$, 2, $\pi$) | (5.9, 6.1, 0.1, 2.9)            | 0.13        | 45                       | 32   |
| 550        | 11180  | 128 | 257 | (2$\pi$, 2, $\pi$) | (9.0, 6.7, 0.04, 4.5)           | 0.04        | 12                       | 64   |
| 950        | 20580  | 128 | 385 | ($\pi$, 2, $\pi$/2) | (7.8, 7.6, 0.03, 3.9)           | 0.02        | 7                        | 64   |

where $u_k^a$ is the spectral component of wavenumber vector $k$, for the velocity component of index $a$. The term $f_0^a(k, t)$ are the spectral coefficients of $f_0^a$, the Navier-Stokes linear operator is given by $D_0^a(k)$, and $K^{abc}(k, k', k'')$ are the nonlinear interaction coefficients. The structure of (3) holds for any form of scale space decomposition, with only the specific form of the coefficients differing. The interaction coefficients for three-dimensional Fourier discretisation are detailed in [24]. In the present study the flow variables are discretised using a Fourier discretisation in $x$ of wavenumber $\alpha$, a collocated Chebyshev discretisation in $y$ of polynomial index $j$, and a Fourier discretisation in $z$ of wavenumber $\beta$. We define our pseudo wavenumber vector to be $k \equiv (k_1, k_2, k_3) \equiv (\alpha, j, \beta)$. Note that $u_k^a(t) = u_{-k}^a(t)$, where the superscript $*$ is the complex conjugate operation and $-k = (-\alpha, j, -\beta)$. The specific form of $D_0^a(k), K^{abc}(k, k', k'')$ and $f_0^a(k, t)$ can be deduced from [34]. The DNS is solved over the rectangular wavenumber and Chebyshev polynomial set of maximum DNS truncation wavenumber $T$, and truncation Chebyshev polynomial index $N$. The summations immediately after the equals sign in (3) are over the wavenumber set

$$T = \{k' : \abs{k'} \leq T, \abs{k'}^2 \leq N, -T \leq k_3' \leq T, 0 \leq k_1'' \leq T, 0 \leq k_2'' \leq N, -T \leq k_3'' \leq T\}.$$ (4)

Note that the mechanics of the channel code are such that it solves for the prognostic variables: $\zeta$, the wall-normal vorticity; and $\nabla^2 u$, where $\nabla^2$ is the Laplacian operator [34]. The evolution of the velocity field, however, is still governed by (3). Finally unless otherwise stated, all quantities presented within are nondimensionalised by the channel half-height $h$, and the freestream centreline velocity $u_0$. We undertake simulations at three friction-velocity-based Reynolds numbers of $Re_\tau \equiv u_\tau h/\nu = 180, 550$ and 950, where the friction velocity $u_\tau = \sqrt{\tau_{wall}/\rho}$ with $\tau_{wall}$ the magnitude of the wall shear stress. In the present simulations the channel flow is simulated in a rectangular box of streamwise extent $L_x$, wall-normal extent $L_y$, and spanwise extent $L_z$, with respective grid collocated points in each direction of $N_x = N_y = N$ and $N_z$. The number of grid points in the horizontal directions is related to the dealised truncation wavenumber $T$ by $N_x = N_z = 3T$. The grid properties for each of the simulations are listed in Table 1, along with the LES truncation resolutions calculated from each DNS. Grid spacings are also presented in viscous units, denoted by the superscript $^+$, where they are nondimensionalised by the length scale $\nu/u_\tau$. The constant grid spacing in the streamwise and spanwise directions in viscous units is given by $\Delta x^+$ and $\Delta z^+$ respectively. In the wall-normal direction, the minimum grid spacing is located at the wall ($\Delta y_{wall}^+$), and the maximum grid spacing is located at the channel centreline ($\Delta y_{cl}^+$). For completeness Table 1 also includes the constant time-step size ($\Delta t$) used in the each of the
For all $Re_\tau$ the: (a) time-averaged streamwise velocity in viscous units $\bar{u}^+$, with key also applicable to (b); and (b) rms streamwise velocity in viscous units $u_{rms}^+$. (c) Instantaneous iso-surfaces of the discriminant of the velocity-gradient tensor equal to unity, coloured by streamwise vorticity with red positive rotation and blue negative rotation.

Simulations presented in viscous units ($\Delta t^+ = \Delta t u_*/h$), and the number of flow-through times over which the statistics are accumulated given by $(t_f - t_i)L_x/u_0$, where $t_f$ and $t_i$ are the final and initial times respectively.

For all three $Re_\tau$ cases we plot the statistical velocity profiles in Fig. 1. Firstly we decompose the instantaneous velocity field, $u$, into its time-averaged mean $\bar{u}$, and its fluctuating component $\hat{u}$. The velocity field is scaled into viscous units given by $u^+ \equiv u/u_*$. Time-averaged and root-mean-square (rms) streamwise velocity profiles are plotted in Fig. 1(a) and Fig. 1(b) respectively. All of the statistical profiles are consistent with previous DNS [35]. We also illustrate the instantaneous flow field of the $Re_\tau = 180$ case in Fig. 1(c), via iso-surfaces of the discriminant of the velocity gradient tensor equal to one. The iso-surfaces are coloured by streamwise vorticity, where red is positive rotation and blue negative rotation about the streamwise axis. The flow is left to right, with the walls indicated by the grey boundaries. We will now apply the SE subgrid modelling approach to these DNSs.

3. Stochastic self-energy modelling of the subgrid scales
The stochastic SE modelling approach developed in [27] is used to model the interactions between resolved and subgrid eddies and hence represent the transfer of energy between them. As discussed in section 2 the DNS is simulated over the complete wavenumber set $T$ of truncation wavenumber $T$ and truncation Chebyshev polynomial index $N$. In the present study we decompose the scales of motion using a rectangular truncation, where the resolved wavenumber set is defined by

$$R = \{ k', k'' \mid 0 \leq k'_1 \leq T_R \, , \, 0 \leq k'_2 \leq N \, , \, -T_R \leq k'_3 \leq T_R \\
0 \leq k''_1 \leq T_R \, , \, 0 \leq k''_2 \leq N \, , \, -T_R \leq k''_3 \leq T_R \} ,$$

where $T_R < T$ is the LES truncation wavenumber. Recall that $k \equiv (k_1, k_2, k_3) \equiv (\alpha, j, \beta)$. Note that we keep all of the Chebyshev polynomials, maintaining all of the vertical scales, and hence consider only the effect of the removal of the horizontal scales. The subgrid wavenumber set is then defined as $S = T - R$.

To facilitate the following discussion on how the subgrid interactions are represented, we introduce a general state vector $q$ of length $N_q$. There are several options for defining the specific form of $q$, which will be discussed at the end of this section. Firstly the tendency (time derivative) of $q$ is decomposed such that

$$q_t(t) = q_R^R(t) + q_S^S(t) .$$
The tendency of the resolved scales is \( q^R_t \), where all triadic interactions involve wavenumbers within the resolved set \( R \). The remainder is the subgrid tendency, \( q^S_t \), which has at least one wavenumber within the subgrid set \( S \) involved in the triadic interactions. In its most primitive form, the subgrid modelling problem is the determination of the relationship between \( q^S_t \) and \( q \) within the resolved set \( R \). The subgrid tendency is further decomposed by

\[
q^S_t(t) = \hat{T} + \hat{q}^S(t),
\]

where \( \hat{T} = \langle q^S \rangle \) is the time-averaged subgrid tendency, and \( \hat{q}^S \) the fluctuating component. The \( \hat{q}^S \) term represents the eddy-eddy subgrid tendency, and in the absence of surface roughness \( \hat{T} \) represents the summation of the eddy-meanfield and meanfield-meanfield interactions. One can decompose these interaction types using the process outlined in [36]. In the current work the values of \( \langle q^S \rangle \) are determined directly from the DNS, and \( \hat{q}^S \) is modelled.

The fluctuating component of the subgrid tendency, \( \hat{q}^S \), is represented by the stochastic equation

\[
\hat{q}^S(t) = -D_d \hat{q}(t) + \hat{f}(t),
\]

where \( D_d \) is the subgrid drain dissipation matrix, \( \hat{q} \) is the fluctuating component of \( q \), and \( \hat{f} \) is a random forcing vector. The matrix \( D_d \) is a time-independent \( N_q \times N_q \) matrix, and \( \hat{f} \) is a time-dependent \( N_q \) element column vector. The drain dissipation operator is determined by post-multiplying both sides of (8) by \( \hat{q}^\dagger (t_0) \), integrating over the turbulent decorrelation period \( \tau \), and ensemble averaging. The expression for \( D_d \) is based on a generalisation of Gauss’s theorem of least squares and given by

\[
D_d = -\left( \int_{t_0}^{t} \hat{q}^S(\sigma)\hat{q}^\dagger(\tau_0)d\sigma \right) \left( \int_{t_0}^{t} \hat{q}(\sigma)\hat{q}^\dagger(\tau_0)d\sigma \right)^{-1},
\]

where \( \dagger \) denotes the Hermitian conjugate for vectors and matrices. The angled brackets denote ensemble averaging, with each ensemble member determined by shifting the initial time \( t_0 \) and the final time \( t = t_0 + \tau \) forward by one time step. For the present data \( D_d \) increases and eventually plateaus with increasing \( \tau \), as previously observed for atmospheric and oceanic flows [31, 32]. We present \( D_d \) using a value of \( \tau \) that maximises the dissipation, and hence captures the memory effects of the subgrid interactions. The value of \( \tau \) at which \( D_d \) plateaus changes with resolution and Reynolds number, however, in all of the cases presented within \( \tau \) is of the order of \( 100d_t \).

The model for \( \hat{f} \) is determined by calculating the non-linear noise covariance matrix \( F_b = F_b + F_b^\dagger \), where \( F_b = \langle \hat{f}(t) \hat{q}^\dagger(t) \rangle \). By again post-multiplying both sides of (8) by \( \hat{q}^\dagger(t_0) \), and adding the conjugate transpose of (8) pre-multiplied by \( \hat{q}(t_0) \) yields the Lyapunov (or balance) equation

\[
\langle \hat{q}^S(t)\hat{q}^\dagger(t) \rangle + \langle \hat{q}(t)\hat{q}^S(\tau) \rangle = -D_d \langle \hat{q}(t)\hat{q}^\dagger(t) \rangle - \langle \hat{q}(t)\hat{q}^\dagger(t) \rangle D_d + F_b.
\]

Given that \( D_d \) is known, \( F_b \) can now be calculated. From (10) it is clear that there is a balancing act between the deterministic (\( D_d \)) and stochastic (\( F_b \)) components of the subgrid model. As \( D_d \) is dependent upon \( \tau \), it is \( \tau \) that defines this balance. At this point the formulation is general, and \( \hat{f} \) is coloured noise. For the implementation of the stochastic subgrid parameterisation, \( \hat{f} \) is represented as a white noise process such that \( \langle \hat{f}(t) \hat{f}(t') \rangle = F_b \delta(t - t') \). An eigenvalue decomposition of \( F_b \) is then used to produce a stochastic model for \( \hat{f} \), as detailed in [28].

As outlined in (8) the fundamental form of subgrid turbulence is a stochastic process, comprising of the deterministic drain dissipation and a stochastic backscatter force. However,
one can approximate the subgrid interactions by a solely deterministic relationship \( \hat{q}^S(t) = -D_{\text{net}} \hat{q}(t) \), where \( D_{\text{net}} \) is the net dissipation representing the net effect of the drain and backscatter [27]. The net dissipation is given by

\[
D_{\text{net}} = D_d + D_b = -\left\langle \hat{q}^S(t) \hat{q}^T(t) \right\rangle - \left\langle \hat{q}(t) \hat{q}^T(t) \right\rangle^{-1}, \quad \text{where} \quad \left(11\right)
\]

is the backscatter dissipation. From (11) it is clear that \( D_{\text{net}} \) is independent of \( \tau \). The drain, backscatter and net eddy viscosities are respectively given by \( \nu_d \equiv D_d \nabla^{-2}, \nu_b \equiv D_b \nabla^{-2}, \) and \( \nu_{\text{net}} \equiv D_{\text{net}} \nabla^{-2}. \)

As all of the subgrid matrices discussed above have dimensions \( N_q \times N_q \), it is advisable to minimise the size of \( q \). In the most general case, \( q \) would contain all of the spectral components of all field variables. For our present rectangular truncation, with the state vector containing all three velocity components, \( N_q = 3T_R^2 N \), which at reasonable resolution is clearly too large for the SE subgrid approach to be tractable. One can reduce the dimension of the problem, however, by adopting the approach undertaken in the QDIA closure developed in [33]. This study formally showed that the subgrid tendency \( q^S \) at a particular wavenumber (or pair, or triplet depending on the number of scale decomposed directions) can be renormalised to be a function of the resolved field \( q \) at only that same wavenumber. This approach was successfully applied to spherical QG atmospheric simulations in [28], producing resolution independent LES. The QDIA assumption was applied in the horizontal periodic directions, with the full matrix form used in the vertical. In this study there was one flow variable and two vertical levels, which meant that \( N_q = 2 \). Using this approach for the channel flow, for each wavenumber pair \((\alpha, \beta)\) we have a state vector \( q(\alpha, \beta, t) \) containing the Chebyshev coefficients of each of the three variables, with \( N_q = 3N \). This may well be tractable but still introduces a significant issue concerning the sampling of the off-diagonal elements of the subgrid matrix statistics. We can take one step further, however, by also applying the QDIA approach in the wall-normal direction. We apply the approach in a pseudo-scale space by factorising the problem in terms of the Chebyshev polynomial indices \( j \). Now for each \( k \equiv (\alpha, j, \beta) \) the state vector takes the form

\[
q(k, t) = [u(k, t), v(k, t), w(k, t)]^T, \quad \text{(13)}
\]

where \( q \) is now of length \( N_q = 3 \). This allows the subgrid scale model to be applied locally to each wavenumber pair and Chebyshev polynomial index, whilst still capturing the coupling between the three velocity components. The subgrid coefficients in this form are illustrated in section 4.

4. Subgrid eddy viscosities in scale space

In this section we present the subgrid coefficients for each of the \( Re_c = 180, 550 \) and 950 channel flows using a rectangular truncation in the two periodic horizontal directions, as outlined in (5). The subgrid interactions are assumed quasi-diagonal in both Fourier and Chebyshev polynomial space as presented in (13).

We initially present the subgrid coefficients for the \( Re_c = 180 \) truncated back to \( T_R = T/2 = 32 \). The subgrid net dissipation matrix elements are illustrated in Fig. 2. They are plotted in the horizontal wavenumber plane \((\alpha, \beta)\) for Chebyshev polynomial index \( j = 41 \), with an effective wall-normal scale of \( \lambda^+ = 2 \), where \( \lambda^+_y = \lambda_y Re_c \). We define \( \lambda_y \) to be the distance between the wall and the second turning point of the \( j \)-th polynomial index, given by \( 1 - \cos(2\pi/j) \). The matrix elements \( D_{\text{net}}^{uv} \) can be interpreted as the transfer function linking the resolved velocity field \( v \) to the subgrid tendency of velocity component \( u \), and likewise for the other matrix
components. It is clear from Fig. 2 that at this particular truncation level \( T_R = T/2 = 32 \), the diagonal components are dominant. This means the subgrid tendency for a given velocity component is most strongly related to the resolved field of the same velocity component. The diagonal elements are also positive throughout the wavenumber plane which means energy is being drained out of the resolved scales and sent to the subgrid. The dissipations are also scale selective with the magnitude of the coefficients increasing as they approach the truncation boundaries. This means that the small resolved vortices near truncation have more significant interactions with the subgrid than the larger resolved structures. This is a typical phenomena and has previously been observed in the associated subgrid coefficients in atmospheric and oceanic simulations [31, 32].

The picture becomes somewhat more complicated, however, when inspecting the other Chebyshev polynomials. We concentrate for the moment on the \( D_{ uu}^{\text{net}} \) term. This element is symmetric about the line \( \beta = 0 \), so we only plot these coefficients in the wavenumber half-plane \((\alpha, \beta \geq 0)\). The \( D_{ uu}^{\text{net}} \) coefficients are illustrated for \( \lambda_y/h = 0.1 \), \( \lambda_y^+ = 2 \), \( \lambda_y^+ = 10 \), and \( \lambda_y^+ = 0.5 \) in Fig. 3(a)-(d) respectively. The \( D_{ uu}^{\text{net}} \) coefficients for \( \lambda_y/h = 0.1 \) and \( \lambda_y^+ = 10 \) have qualitatively the same properties for as \( \lambda_y^+ = 2 \) discussed above. For \( \lambda_y^+ = 0.5 \), however, the smallest resolved scales in the top right hand corner of Fig. 3(l) have negative net dissipations. This indicates that the subgrid interactions are conspiring to send energy from the subgrid to these wavenumber pairs, representative of a backscatter of energy. One can determine if this backscatter is coherent or incoherent by decomposing the net dissipation into its deterministic and stochastic components. The deterministic drain dissipation \( D_{ uu}^{\text{dr}} \) is illustrated for the same Chebyshev polynomial indices in Fig. 3(e)-(h), with the associated stochastic backscatter dissipation \( D_{ uu}^{\text{bs}} \) illustrated in Fig. 3(i)-(l). In all cases the drain dissipation is completely positive.

![Figure 2](image-url)

**Figure 2.** Subgrid net dissipation matrix elements for the \( Re_T = 180 \) case, illustrated in the horizontal wavenumber half-plane \((\alpha, \beta \geq 0)\) at \( \lambda_y^+ = 2 \), using rectangular truncation with \( T_R = T/2 = 32 \): (a) \( D_{ uu}^{\text{NET}} \); (b) \( D_{ uu}^{\text{DD}} \); (c) \( D_{ uu}^{\text{DB}} \); (d) \( D_{ uu}^{\text{BS}} \); (e) \( D_{ uu}^{\text{BS}} \); (f) \( D_{ uu}^{\text{BS}} \); (g) \( D_{ uu}^{\text{BS}} \); (h) \( D_{ uu}^{\text{BS}} \); and (i) \( D_{ uu}^{\text{BS}} \). The colour bars in the final column are the same and applicable to all figures.
and the stochastic backscatter completely negative. This means that energy is sent from the resolved to the subgrid scales in a deterministic coherent manner, and energy is sent from the subgrid to the resolved in an incoherent stochastic manner. It is only at the smallest vertical scales that the stochastic backscatter overwhelms the drain dissipation resulting in negative net dissipation in Fig. 3(d) for certain wavenumber pairs.

The higher $Re_{\tau}$ cases have similar properties. The same $D_{\text{uu}}^{\text{net}}$ are plotted for the $Re_{\tau} = 180$ case in Fig. 4(a)-(d). They are lined up with coefficients from $Re_{\tau} = 550$ in Fig. 4(e)-(h) and $Re_{\tau} = 950$ in Fig. 4(i)-(l) with the same vertical scales. These figures illustrate that as $Re_{\tau}$ increases so too does the magnitude of $D_{\text{uu}}^{\text{net}}$. For each $Re_{\tau}$, the $D_{\text{uu}}^{\text{net}}$ coefficients for $\lambda_y^+ = 0.5$ contain negative values for certain wavenumber pairs, indicating that energy is sent to these wavenumbers from the subgrid. Inspection of the associated drain and stochastic backscatter dissipations (not shown) indicates that the injection of energy is again stochastic in nature. Current work is looking to identify a potential universal scaling of these coefficients.

5. Subgrid eddy viscosities in horizontal scale and vertical physical space

So far we have presented the subgrid dissipations diagonalised based on horizontal and vertical scale, and identified that there is a net injection of energy into the smallest resolved vertical
Figure 4. The net dissipation matrix element $D_{uu}^{\text{net}}$ illustrated in the horizontal wavenumber half-plane $(\alpha, \beta \geq 0)$ using rectangular truncation $T_R = T/2$ for various Chebyshev polynomials (index $j$) with characteristic wall-normal scale $\lambda_y = 1 - \cos(2\pi/j)$. The first row (a)-(d) contains the $Re_\tau = 180$ case. The second row (e)-(h) contains the $Re_\tau = 550$ case. The third row (i)-(l) contains the $Re_\tau = 950$ case. In the first column (a),(e),(i) $\lambda_y/h = 0.1$. In the second column (b),(f),(j) $\lambda_y/h = 10$. In the third column (c),(g),(k) $\lambda_y/h = 2$. In the fourth column (d),(h),(l) $\lambda_y/h = 0.5$. All coefficients are symmetric about the line $\beta = 0$. The colour bars in the final column are applicable to all figures in that row.

scales (large Chebyshev polynomial index $j$). It is not clear, however, where in physical space this injection of energy is occurring. However, we can identify the regions of injection by looking at the subgrid interactions on the basis of vertical position instead of vertical scale. Whilst the subgrid interactions are quasi-diagonal in scale space, inspecting the structure of the subgrid dissipations diagonalised based on vertical position can also provide some insight.

The associated $D_{uu}^{\text{net}}$ coefficients are plotted for each of the $Re_\tau$ cases in Fig. 5 at four different wall-normal positions of $y = 1$ (centreline), $y = 0.5$, $y^+ = 10$ and $y^+ = 1$. The net dissipations at each of these positions for the $Re_\tau = 180$ case are illustrated in Fig. 5(a)-(d), for $Re_\tau = 550$ in Fig. 5(e)-(h), and $Re_\tau = 950$ in Fig. 5(i)-(l). In all cases energy is drained out of the system in the body of the channel, with there being a net injection of energy at a wall-normal position of $y^+ = 1$. The magnitude of the dissipations again increase with $Re_\tau$.

These observations are consistent with the physical view of wall-bounded turbulence. In the attached eddy hypothesis of [37] spanwise vorticity generated at the wall in the form of spanwise oriented vortex lines are lifted up and elongated in the streamwise direction by the mean flow. These wall-attached eddies of small vertical and horizontal scale, transfer energy to larger wall-attached eddies with their centreline located at a slightly greater distance from the wall, leading to a form of inverse energy cascade [38, 39, 40, 41, 42]. Truncating the DNS by removing the small horizontal scales removes the source of energy injection in the system (the
Figure 5. The net dissipation matrix element $D_{\text{net}}^{uu}$, illustrated in the horizontal wavenumber half-plane ($\alpha, \beta \geq 0$) using rectangular truncation $T_R = T/2$ for various wall-normal positions $y$. The first row (a)-(d) contains the $Re_{\tau} = 180$ case. The second row (e)-(h) contains the $Re_{\tau} = 550$ case. The third row (i)-(l) contains the $Re_{\tau} = 950$ case. In the first column (a),(e),(i) $y = 1$. In the second column (b),(f),(j) $y = 0.5$. In the third column (c),(g),(k) $y^+ = 10$. In the fourth column (d),(h),(l) $y^+ = 1$. All coefficients are symmetric about the line $\beta = 0$. The colour bars in the final column are applicable to all figures in that row.

wall-attached eddies). This injection of energy is represented by the negative net coefficients of the small vertical scales illustrated in Fig. 4, and also at small wall-normal distance as illustrated in Fig. 5. At some point the initially wall-attached eddies detach themselves from the wall. The now detached eddy breaks down into smaller eddies giving rise to a forward energy cascade [38, 39, 40, 41, 42]. This dissipation of energy is represented by the positive net coefficients for larger vertical scales and wall-normal positions.

6. Large eddy simulation

In this section we will illustrate the ability of LESs of the $Re_{\tau} = 180$ case to replicate the spectra of the associated DNS. As discussed in section 3, LESs can be undertaken using either a stochastic or a deterministic subgrid parameterisation. The equations governing the LES are the same as for the DNS, but with $q^S(k)$ added to the right-hand-side of the prognostic equations, and solved over the wavenumber set $R$ instead of $T$. Recall that $k \equiv (\alpha, j, \beta)$. In the stochastic representation $q^S(k)$ is given by the following matrix equation

$$q^S(k, t) = -D_d(k) \tilde{q}(k, t) + \tilde{f}(k, t) + \bar{f}(k),$$

where the eddy-meanfield terms, $\bar{f}$, are also those determined from the DNS. In the deterministic LES the drain dissipation and stochastic backscatter are replaced with the net dissipation, $D_{\text{net}}$,.
such that

\[ q_S^S(k,t) = -D_{\text{net}}(k) \hat{q}(k,t) + \tilde{f}(k) \]  \hspace{1cm} (15)

On a technical matter, recall the channel code solves for the flow field on the basis of the state vector \((\zeta, \nabla^2 v)\), however, to facilitate physical interpretation of the results the subgrid parameterisations were developed on the basis of the velocity components. For the implementation of the LES, the same channel code is run at reduced resolution again solving for \((\zeta, \nabla^2 v)\). At each time step the Poisson equation is solved to convert the instantaneous \((\zeta, \nabla^2 v)\) to the velocity components \((u, v, w)\). The subgrid model is then applied to the instantaneous resolved velocity field to produce the associated subgrid tendency in velocity space \((u_S^S, v_S^S, w_S^S)\). The subgrid tendency is then converted back to \((\zeta_S^S, \nabla^2 v_S^S)\) and added to the right-hand-side of the DNS equations.

Comparisons between the DNS and LES are made at various wall-normal positions, on the basis of the time-averaged spanwise wavenumber summed kinetic energy spectra as a function of streamwise wavenumber. In all of the following plots the DNS is represented by the dashed lines, and the LES by the solid lines. The pairs of spectra are labelled by the associated value of \(y^+\) with each pair shifted down multiples of one decade from the top pair for clarity. Firstly to serve as a baseline comparison, we truncate the DNS to the LES resolution of \(T_R = T/2 = 31\) with no subgrid model prescribed. The resulting spectra are compared to the DNS spectra in Fig 6(a). This clearly illustrates an accumulation of energy at the smallest resolved scales of motion because the now unresolved subgrid interactions would have drained this energy out of the resolved scales and into the subgrid. This accumulation of energy can be alleviated by adopting either of the deterministic or stochastic SE subgrid models. The kinetic energy spectra of the deterministic LES, using the subgrid model defined in (15), is compared to the DNS spectra in Fig 6(b). Likewise the kinetic energy spectra of the stochastic LES, using the subgrid model defined in (14), is compared to the DNS spectra in Fig 6(c). Both the deterministic and stochastic implementations of the SE subgrid model are able to correct the kinetic energy spectra and reproduce the DNS statistics. This high level of agreement indicates that the deterministic and stochastic SE subgrid models accurately represent the subgrid interactions. It is, therefore, valid to make physical interpretations of the energy transfers from the sign, magnitude and spectral dependence of the SE subgrid model coefficients.
7. Concluding remarks and future applications

Self-energy subgrid models have been developed for turbulent channel flows. The stochastic parameterisation of the eddy-eddy interactions consists of a drain dissipation, and a stochastic backscatter noise term. The deterministic version is governed solely by the net dissipation, representing the net effect of the drain and backscatter. These subgrid matrices are functions of the streamwise and spanwise wavenumbers and the Chebyshev polynomial index, and explicitly capture the interactions between each of the three velocity components. These scale dependent matrices have been derived from the statistics of higher resolution DNSs. LESs adopting the stochastic and deterministic subgrid models diagonalised on the basis of horizontal and vertical scale were successful in replicating the statistics of the DNS.

Inspection of the three-dimensional scale-based net eddy viscosities indicates that the removal of small horizontal scales results in a net drain of energy out of the system for the large vertical scales, and an injection of energy to the smallest resolved vertical scales. Decomposing the net eddy viscosity into the drain and backscatter components, illustrates that the injection of energy is a stochastic one. Diagonalising the subgrid interactions on the basis of vertical position instead of vertical scale identified that the injection of energy was concentrated in the near wall region for all Reynolds numbers. This is consistent with the attached eddy hypothesis [37, 38] stating that small wall-attached eddies transfer energy to larger wall-attached eddies giving rise to an inverse energy cascade, and upon detachment break down into smaller eddies giving rise to a forward energy cascade [41, 42]. In the framework presented here, the inverse cascade is represented by the negative net dissipations, and the forward cascade is represented by the positive net dissipations.

These findings may also have implications for the development of wall models. First and foremost a wall model must apply an appropriate boundary condition at the first grid point away from the wall, as illustrated in [43, 5, 44, 45, 46, 47]. However, in the present study it has been identified that the removal of small wall-attached eddies results in a net injection of energy to the larger resolved eddies. Ideally, in addition to applying the correct boundary condition, wall models should also represent this injection of energy and the necessary dampening. The SE approach presented in this paper could be used to determine the complete structure of a wall model by decomposing the resolved and subgrid scales on the basis of vertical scale (or potentially position). Depending on the complexity of the resulting subgrid coefficients, the eddy viscosities may then be represented in a more simple form in order to construct a more general purpose wall model, complementing the application of the appropriate boundary conditions. The extent to which such an approach would improve current wall modelling efforts is an open question.

The SE subgrid modelling approach is initially computationally expensive as a DNS must be run to determine the subgrid coefficients. However, because no physical assumptions are made in the development of the model, physical interpretations can be made from the subgrid coefficients concerning the energy transfers between the resolved and subgrid scales. In the present work we decompose the resolved and subgrid horizontal scales in a rectangular manner in wavenumber space consistent with the spectral discretisation of the DNS. However, one could also truncate on the basis of an effective horizontal wavenumber $k_{2D} = \sqrt{\alpha^2 + \beta^2}$, and define the resolved scales as all wavenumber pairs with $k_{2D}$ less than a threshold horizontal LES truncation wavenumber. Truncating the system in this form may be more amenable to representing the eddy viscosities by a set of broadly applicable scaling laws, as has been previously undertaken for atmospheric [31] and oceanic flows [32]. This would then remove the need to generate the eddy viscosities from a reference DNS. Additionally one could identify the effect of removing specific vortex structures defined by a certain wavenumber set – for example removing spectral components representative of streamwise oriented streaks, or any other type of flow structure for that matter. The work presented here paves the way for many research opportunities in a vast array of configurations, not only channel flows, and also not only fluid mechanics. In fact the approach is applicable to
any classical nonlinear multi-scale system [33, 24].

Acknowledgments
The authors would like to acknowledge the co-funding of this research by the European Research Council via the 2013 Multiflow summer program, the Australian Research Council, and the Commonwealth Scientific and Industrial Research Organisation. The authors would also like to thank Dr Ricardo García-Mayoral for his feedback during the development of the manuscript.

References
[1] Smagorinsky J 1963 General circulation experiments with the primitive equations: I. The basic experiment Mon. Wea. Rev. 91 99–164
[2] Germano M, Piomelli U, Moin P and Cabot WH 1991 A dynamic subgrid-scale eddy viscosity model Phys. Fluids A 3 1760–1765
[3] Lilly DK 1992 A proposed modification of the Germano subgrid-scale closure method Phys. Fluids A 4 633–635
[4] Misra A and Pullin DI 1997 A vortex-based subgrid stress model for large-eddy simulation Phys. Fluids 9 2443–2454
[5] Chung D and Pullin DI 2009 Large-eddy simulation and wall modelling of turbulent channel flow J. Fluid Mech. 631 281–309
[6] McComb WD, Hunter A and Johnson C 2001 Conditional mode elimination and the subgrid-modelling problem for isotropic turbulence Phys. Fluids 13 2030–2044
[7] Kraichnan RH 1959 The structure of isotropic turbulence at very high Reynolds numbers J. Fluid Mech. 5 497–543
[8] Herring JR 1965 Self consistent field approach to turbulence theory Phys. Fluids 8 2219–2225
[9] McComb WD 1974 A local energy-transfer theory of isotropic turbulence J. Phys. A: Math. Gen. 7 632–649
[10] McComb WD 1990 The Physics of Fluid Turbulence (Clarendon Press, Oxford)
[11] Carnevale GF and Frederiksen JS 1983 Viscosity renormalization based on direct-interaction closure J. Fluid. Mech. 131 289–303
[12] Frederiksen JS, Davies AG and Bell RC 1994 Closure theories with non-Gaussian restarts for truncated two-dimensional turbulence Phys. Fluids 6 3153–3163
[13] Kiyani K and McComb WD 2004 Time-ordered fluctuation-dissipation relation for incompressible isotropic turbulence Phys. Rev. E 70 066303
[14] Kraichnan RH 1976 Eddy viscosity in two and three dimensions J. Atmos. Sci. 33 1521–1536
[15] Leslie DC and Quarini GL 1979 The application of turbulence theory to the formulation of subgrid modelling procedures J. Fluid Mech. 91 65–91
[16] Chollet JP and Lesieur M 1981 Parameterization of small scales of three-dimensional isotropic turbulence utilizing spectral closures J. Atmos. Sci. 38 2747–2757
[17] Leith CE 1990 Stochastic backscatter in a subgrid-scale model: Plane shear mixing layer Phys. Fluids 2 297–299
[18] Chasnov JR 1991 Simulation of the Kolmogorov inertial subrange using an improved subgrid model Phys. Fluids A 3 188–200
[19] Domaradzki JA, Liu W and Brachet ME 1993 An analysis of subgrid scale interactions in numerically simulated isotropic turbulence Phys. Fluids A 5 1747–1759
[20] McComb WD and Johnson C 2001 Conditional mode elimination and scale-invariant dissipation in isotropic turbulence Physica A 292 346–382
[21] Frederiksen JS and Davies AG 1997 Eddy viscosity and stochastic backscatter parameterizations on the sphere for atmospheric circulation models J. Atmos. Sci. 54 2475–2492
[22] Frederiksen JS 1999 Subgrid-scale parameterizations of eddy-topographic force, eddy viscosity and stochastic backscatter for flow over topography J. Atmos. Sci. 56 1481–1493
[23] O’Kane TJ and Frederiksen JS 2008 Statistical dynamical subgrid-scale parameterizations for geophysical flows Phys. Scr. T132 014033
[24] Frederiksen JS 2012 Self-energy closure for inhomogeneous turbulence and subgrid modeling Entropy 14 769–799
[25] Schwinger J 1948 Quantum electrodynamics. I: A covariant formulation Phys. Rev. 74 1439–1461
[26] Berera A, Salewski M and McComb WD 2013 Eulerian field-theoretic closure formalisms for fluid turbulence Phys. Rev. E 87 013007
[27] Frederiksen JS and Kepert SM 2006 Dynamical subgrid-scale parameterizations from direct numerical simulations J. Atmos. Sci. 63 3006–3019

[28] Zidikheri MJ and Frederiksen JS 2009 Stochastic subgrid parameterizations for simulations of atmospheric baroclinic flows J. Atmos. Sci. 66 2844–2858

[29] Zidikheri MJ and Frederiksen JS 2010 Stochastic modelling of unresolved eddy fluxes Geophys. Astrophys. Fluid Dyn. 104 323–348

[30] Zidikheri MJ and Frederiksen JS 2010 Stochastic subgrid-scale modelling for non-equilibrium geophysical flows Phil. Trans. Royal Soc. A 368 145–160

[31] Kitsios V, Frederiksen JS and Zidikheri MJ 2012 Subgrid model with scaling laws for atmospheric simulations J. Atmos. Sci. 69 1427–1445

[32] Kitsios V, Frederiksen JS and Zidikheri MJ 2012 Scaling laws for parameterisations of subgrid eddy-eddy interactions in simulations of oceanic circulations Ocean Modelling 68 88–105

[33] Frederiksen JS 2012 Statistical dynamical closures and subgrid modeling for inhomogeneous QG and 3D turbulence Entropy 14 32–57

[34] Kim J, Moin P and Moser R 1987 Turbulence statistics in fully developed channel flow at low Reynolds number J. Fluid Mech. 177 133–166

[35] Del Álamo JC and Jiménez J 2003 Spectra of the very large anisotropic scales in turbulent channels Phys. Fluids 15 L41–L44

[36] Kitsios V, Frederiksen JS and Zidikheri MJ 2013 Subgrid parameterisation of the eddy-meanfield interactions in a baroclinic quasi-geostrophic ocean ANZIAM J. 54 C304–C410

[37] Townsend AA 1961 Equilibrium layers and wall turbulence J. Fluid. Mech. 11 97–120

[38] Perry AE and Chong MS 1982 On the mechanism of wall turbulence J. Fluid. Mech. 119 173–217

[39] Lozano-Durán A and Jiménez J 2011 Time-resolved evolution of the wall-bounded vorticity cascade J. Phys.: Conf. Series 318 062016

[40] Lozano-Durán A, Flores O and Jiménez J 2012 The three-dimensional structure of momentum transfer in turbulent channels J. Fluid. Mech. 694 100–130

[41] Cimarelli A and de Angelis E 2012 Anisotropic dynamics and sub-grid energy transfer in wall-turbulence Phys. Fluids 24 015102

[42] Cimarelli A, de Angelis E and Casciola CM 2013 Paths of energy in turbulent channel flows J. Fluid. Mech. 715 436–451

[43] Piomelli U and Balaras E 2002 Wall-layer models for large eddy simulation Annu. Rev. Fluid Mech. 34 349–74

[44] Marusic I, Mathis R and Hutchins N 2010 Predictive model for wall-bounded turbulent flow Science 329 193–196

[45] Podvin B and Fraigneau Y 2011 Synthetic wall boundary conditions for the direct numerical simulation of wall-bounded turbulence J. Turb. 12 1–26

[46] García-Mayoral R, Pierce B and Wallace J 2012 Off-wall boundary conditions for turbulent simulations from minimal flow units in transitional boundary layers CTR Summer Prog. (Stanford Univ.) pp 87–96

[47] Mizuno Y and Jiménez J 2013 Wall turbulence without walls J. Fluid. Mech. 723 429–455