Rapid distortion theory applied to the analysis of under–resolved simulations of turbulent boundary layers

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This paper uses rapid distortion theory (RDT) to study the truncation error in boundary layer simulations at coarse resolution. RDT is applied to homogeneous turbulence under uniform mean shear. The RDT equations are discretized, and the discrete equations are analytically solved. The effect of truncation error on linear, homogeneous turbulence is shown to be similar to that in turbulent channel flow. The RDT equations and the channel results are used to suggest that the dominant source of error arises from the discrete Poisson equation for pressure. This effect is shown to be a result of constraining the velocity field to be divergence–free in the presence of truncation error. The results suggest that possible need to model the effect of the subgrid scales on the non–local effects of pressure near the wall in large–eddy simulation.

1. Introduction

The direct numerical or large–eddy simulation (LES) of attached, wall–bounded flows is prohibitively expensive at high Reynolds numbers (see e.g. Chapman 1979, Moin 1998, Piomelli & Balaras 2002). High Reynolds numbers require exceedingly fine resolution for correct predictions to be obtained. Chapman (1979) provided the first detailed estimate of resolution requirements for large–eddy simulation of wall–bounded flows. The ‘outer layer’ was assumed to be dominated by motions that scaled with the boundary layer thickness and depended on the Reynolds number only through the dependence of the boundary layer thickness on the Reynolds number. The ‘inner layer’ on the other hand was assumed to be dominated by quasi–streamwise vortices (Kline et al. 1967) whose size scaled with wall units ($\nu/u_*$, where $\nu$ and $u_*$ denote the kinematic viscosity and friction velocity respectively). The resolution requirements for the inner layer therefore depend strongly on the Reynolds number. Chapman’s (1979) estimates were used by Reynolds (1990) to estimate that the computational cost varies as $Re^{1/2}$ for the outer layer and $Re^{2.4}$ for the inner layer. Piomelli & Balaras (2002) note that at high Reynolds numbers, most of the increased grid resolution is in the ‘inner layer’; for Reynolds numbers of the order of $10^6$, 99% of the grid points would be used to resolve about 10% of the boundary layer thickness.

The LES methodology assumes that a fraction of the energy–containing motions are resolved on the computational grid. The above discussion implies that this is practical only for lower Reynolds numbers; at very high Reynolds numbers, computationally affordable grids will be so coarse that the inner–layer motions are essentially represented in a Reynolds–averaged sense. Such coarse resolutions preclude integration of the LES equations all the way to the wall. Instead, only the outer layer is resolved on the grid; the
inner layer is modeled through the stresses that it exerts on the outer layer. Piomelli & Balaras (2002) review such ‘wall–layer’ models for LES. They note however that obtaining good predictions using wall–layer models requires that the near–wall resolution be very coarse (greater than 1500 and 700 wall units in the streamwise and spanwise direction). Less accurate predictions are obtained on grids where a fraction of the instantaneous near–wall motions are resolved.

This paper considers the LES modeling of wall–bounded flows where the LES equations are integrated down to the wall. Of particular interest is the question of whether commonly used subgrid models are modeling the dominant physical/numerical effect of the subgrid scales in the inner–layer region. Most subgrid models e.g. Smagorinsky (1963) are conceived for isotropic turbulence, where the subgrid model is required to model the net nonlinear transfer of energy from the resolved scales to the subgrid scales. However, the inner–layer streaks are far from isotropic (Kline et al. 1967). Furthermore, the experiments by Kline et al. and Uzkan & Reynolds (1967), and simulations by Lee et al. (1990) suggest that streaks are produced by the linear mechanism of rapid straining of turbulent fluctuations by the high values of mean shear near the wall.

Lee et al. (1990) consider initially isotropic turbulence that is subjected to homogeneous mean shear. The ratio of time–scales, $S q^2/\epsilon$ was set equal to its peak value ($\sim 35$) in the viscous sublayer of turbulent channel flow at $Re_x = 180$ (Kim et al. 1987). Here, $S$ denotes the mean shear rate, $q^2$ denotes twice the turbulence kinetic energy, and $\epsilon$ denotes turbulent dissipation. It was found that such high shear rates produced streaks in homogeneous turbulence. Also, the nonlinear simulations were shown to be in good agreement with analytical solutions of the linear equations governing the evolution of the fluctuations about the mean homogeneous shear (rapid distortion theory, RDT).

An implication of this past work is that perhaps subgrid models should not model nonlinear energy transfer in the inner layer, but instead should model the linear errors that occur when rapidly sheared turbulence is described using the linear equations. This paper attempts to study these linear errors. Consider rapidly sheared homogeneous turbulence that is numerically solved on a coarse computational mesh. The governing equations are linear and discrete. The resulting numerical error has two components – exclusion of high wavenumber modes, and discretization error in representing the included modes. Note that separation of subgrid–scale and subfilter–scale effects has been recognized in the literature (see e.g. Gullbrand & Chow 2002 and references therein). Classical RDT analysis (e.g. Moffat 1967, Townsend 1970, Rogers 1991) solves the linearized Navier–Stokes equations equations analytically. The classical analysis is easily extended to solve the linear discrete equations analytically. In this process, the effects of truncation error associated with the filtering and the numerical scheme are separately obtained.

The paper is organized as follows. Section 2 shows results from simulations of turbulent plane channel flow on coarse grids. Two widely separated Reynolds numbers are considered, and the qualitative nature of numerical error is shown to be independent of Reynolds number. This behavior is analyzed using rapid distortion theory in section 3, which discusses the governing equations, and details of their numerical solution. The RDT results are shown to be qualitatively similar to the channel flow simulations in section 4, which also provides an explanation for this behavior. The paper concludes with a brief summary in section 5.

2. The effect of grid resolution on near–wall turbulence

The role of truncation error in simulations of wall–bounded flows may be studied by solving the Navier–Stokes equations at coarse resolution. Such simulations were per-
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Table 1. Summary of grids used in the channel flow simulations. The subscript ‘w’ refers to values at the wall.

<table>
<thead>
<tr>
<th>Grid Size</th>
<th>Reynolds Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 x 32 x 16</td>
<td>Re$_x$ = 180</td>
</tr>
<tr>
<td>32 x 32 x 32</td>
<td>Re$_x$ = 1030</td>
</tr>
<tr>
<td>16 x 16 x 16</td>
<td></td>
</tr>
<tr>
<td>96 x 96 x 96</td>
<td></td>
</tr>
</tbody>
</table>

Formed for turbulent plane channel flow at Re$_x$ = 180 and Re$_x$ = 1030. The Re$_x$ = 180 simulations are compared to the DNS results of Kim et al. (1987), while the Re$_x$ = 1030 results are compared to the experiments of Hussain & Reynolds (1970), and Wei & Wilmarth (1989). Note that the friction velocity used in specifying the Reynolds number and normalizing the simulation results, is that obtained from the constant body force ($u^2/h$); at coarse resolutions, it is not equal to the friction velocity obtained from the simulations.

The computational domain was $4\pi \times 2 \times 4\pi/3$ in the streamwise, wall-normal and spanwise direction respectively. A second-order, central-difference, staggered grid formulation (Harlow & Welch 1965) was used for spatial discretization. The third-order Runge–Kutta method (Wray 1986) was used to time-advance all terms, except the viscous terms in the wall-normal direction which were advanced implicitly using the second-order Crank-Nicholson scheme. The computational mesh was uniform in the streamwise and spanwise directions, and non-uniform in the wall-normal direction ($y_j = -\frac{\tanh(\gamma(1-2j)/Ny)}{\tanh \gamma}$). Four computational grids were used, and are described in table 1. The wall-normal stretching parameter, $\gamma$ was 2.8 for all grids. Note that the 16$^3$ grid for the Re$_x$ = 180 computation, and 96$^3$ grid for the Re$_x$ = 1030 computation have the same approximate near-wall spacing in wall units. All simulations used a constant timestep of $\Delta t u_r/h = 0.001$.

Results for the mean velocity and Reynolds stresses are shown in figures 1, 2, and 3 respectively. Note that the nature of the numerical error is similar at both Reynolds numbers. At coarse resolutions, the mean velocity at the centerline is higher, the streamwise
intensity near the wall is higher, and the wall-normal and spanwise turbulence intensities, and the Reynolds shear stress, $u'v'$, are lower than their correct values. Also, even when the mean velocity is reasonably close to the exact solution (e.g. the 32$^3$ grid for the $Re_x = 180$ simulation), the intensities are not. Comparison of the 16$^3$ computation to the other simulations at $Re_x = 180$ suggests that the error need not monotonically approach the correct solution at very coarse resolutions. Also, note that the error in $u'v'$ is directly related to the error in the mean velocity through the mean momentum equation which shows that

$$
\mu \bar{U}(y) = \frac{dP}{dx} \left( \frac{y^2}{2} - hy \right) + \int_0^y u'v' \,dy.
$$

Here, $dP/dx$ denotes the mean pressure gradient which is constant, and $\mu$ denotes the dynamic viscosity. Since $u'v'$ is negative, lower magnitudes increase the centerline velocity in the channel. Coarse grids also affect the location of the peak in $u'v'$. Moving the peak in $u'v'$ away from the wall tends to increase the magnitude of its integral, which decreases the mean centerline velocity. These trends in the Reynolds stresses at coarse resolutions are examined using rapid distortion theory in the following sections.

Figure 2. The effect of grid resolution on $u_{\text{rms}}$ and $v_{\text{rms}}$ at (a) $Re_x = 180$ (--- Kim et al. 1987, - - - - 32$\times$32$\times$32 grid, - - - - 16$\times$32$\times$16 grid,...... 16$\times$16$\times$16 grid ), (b) $Re_x = 1030$ (○ Wei & Wilmarth 1989, □ Hussain & Reynolds 1970, - - - - 32$\times$32$\times$32 grid, - - - - 16$\times$32$\times$16 grid, ...... 96$\times$96$\times$96 grid).
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3. Inviscid Rapid distortion theory

Rapid Distortion Theory combines linearization of the governing equations with statistical averaging to describe the statistical evolution of turbulence under rapid mean distortion (see e.g. the reviews by Savill 1987, and Hunt and Carruthers 1990). When the time-scale of the mean distortion is much smaller than that of the turbulence, then the turbulence has no time to interact with itself. This allows neglect of terms involving the product of fluctuations, and yields equations that are linear in the fluctuations. The analysis may be performed while retaining viscosity (Deissler 1961, Townsend 1976). This paper neglects the viscous terms, since at high Reynolds numbers, the viscous timescale is slower than even the nonlinear turbulence timescale.

Linearization of the continuity and momentum equations yields

\[
\frac{\partial u_i'}{\partial t} + U_j \frac{\partial u_i'}{\partial x_j} + u_j' \frac{\partial U_i}{\partial x_j} = -\frac{\partial p'}{\partial x_i}; \quad \frac{\partial u_i'}{\partial x_i} = 0,
\]

where \( U_i \) denotes the mean velocity, and \( u_i' \) and \( p' \) denote fluctuations in velocity and pressure respectively. Note that \( U_i = A_{ik}(t) x_k \) for homogeneous turbulence.
is solved by changing coordinates to a system that deforms with the mean field (Rogallo 1981); i.e.,
\[ \xi_i = B_{ik}(t)x_k, \quad \tau = t, \]  
(3.2)
where \( \frac{d}{dt} B_{nk} + A_{jk} B_{nj} = 0 \). The coordinate transformation yields linear, constant-coefficient equations which are then solved using conventional Fourier representation. Knowledge of the Fourier coefficients enables computation of the energy spectrum tensor which is then integrated over all wavenumbers to determine the Reynolds stresses.

Note that the wavenumbers vary continuously from \(-\infty\) to \(+\infty\) in an analytical representation of the turbulent field. Two important differences arise when the same problem is numerically solved. First, finite spatial resolution implies that the wavenumbers are finite, and given by \( k_i = \frac{2\pi j}{L} \), where \( j \) varies from \(-N/2\) to \( N/2 - 1 \). Here, \( N \) denotes the number of grid points, and \( L \) denotes the domain size in the \( i \)th direction. Second, discretization error results in the spatial derivatives in the linear equation not being correctly represented. Both factors result in the evolution of the numerical solution being different from the analytical solution.

3.1. Problem statement

Figure 4 shows a schematic of the problem where initially isotropic turbulence is subjected to mean shear. The rate of shear is assumed rapid as compared to characteristic timescales of the turbulence. The mean velocity for homogeneous shear is
\[ U_1 = Sx_2, \quad U_2 = U_3 = 0. \]  
(3.3)
and the corresponding coordinate transformation is \( \xi_1 = x_1 - S\tau x_2, \quad \xi_2 = x_2, \quad \xi_3 = x_3, \quad \tau = t \). Linearizing equation 3.1 about the mean flow in equation 3.3 yields the following equations for the fluctuations:
\[
\begin{align*}
\frac{\partial u'_1}{\partial \tau} + u'_2 S &= - \frac{\partial p'}{\partial \xi_1}, \\
\frac{\partial u'_2}{\partial \tau} &= - \frac{\partial p'}{\partial \xi_2} + S\tau \frac{\partial p'}{\partial \xi_1}, \\
\frac{\partial u'_3}{\partial \tau} &= - \frac{\partial p'}{\partial \xi_3}, \\
\frac{\partial u'_1}{\partial \xi_1} + \frac{\partial u'_2}{\partial \xi_2} - S\tau \frac{\partial u'_2}{\partial \xi_1} + \frac{\partial u'_3}{\partial \xi_3} &= 0.
\end{align*}
\]  
(3.4)

3.2. Numerical solution of the RDT equations

Consider a uniform spatial grid in \( \xi_i \), and discretize equations 3.4 using a finite-difference or finite volume scheme. The discrete equations can be analytically solved as shown below.
Since the turbulence is homogeneous, it may be represented as

\[ u'_x(\xi, \tau) = \sum_k \tilde{u}_i(k, \tau) e^{ik_j \xi_j}, \quad p'(\xi, \tau) = \sum_k \tilde{p}(k, \tau) e^{ik_j \xi_j}. \]  

(3.5)

The number of grid points used, determine the range of resolved wavenumbers in each coordinate direction. Within the resolved range, only a Fourier spectral method computes the spatial derivatives without error. A finite difference or finite volume scheme would have an error which is conveniently represented by the “modified wave-number” (see e.g. Moin 2001).

Consider the periodic function \( f_j = e^{ik_j x_j} \). Its first derivative is \( ik_j e^{ik_j x_j} \). However, a finite-difference or finite volume scheme will yield an expression of the form, \( ik'_j e^{ik_j x_j} \). The variable \( k'_j \) is called the modified wavenumber and depends on \( k \) and the mesh spacing, \( \Delta \). For example, the modified wavenumber for the second order central-difference scheme, \( f'_j = (f_{j+1} - f_{j-1})/2\Delta \) is readily seen to be \( \sin (k\Delta) / \Delta \) (figure 5). The modified wave-number does not have to be a real quantity; it is complex when upwinded spatial difference schemes are used. Note that the modified wavenumber is an analytical solution of the discrete equations on a periodic domain.

An analytical solution to the discrete RDT equations can therefore be obtained. The solution is identical to the classical analytical solutions (e.g. Townsend 1976, Rogers 1991) with the exception that wavenumbers in the analytical solutions are replaced by the modified wavenumber. Note that the solution is completely general in the choice of numerical scheme.

\[ \tilde{u}_1 = \frac{k'^2}{k'^2 + k'^2} C_1(k, \tau) \tilde{u}_2(k, 0) + \tilde{u}_1(k, 0) \]

\[ \tilde{u}_2 = \frac{k'^2}{k'^2 - 2S\tau k'_1 k'_2 + (S\tau k'_1)^2} \tilde{u}_2(k, 0) \]  

(3.6)

\[ \tilde{u}_3 = \frac{k'_1 k'_3}{k'_1^2 + k'_3^2} C_3(k, \tau) \tilde{u}_2(k, 0) + \tilde{u}_1(k, 0) \]
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Figure 6. The evolution of the Reynolds stresses (normalized by the initial value of $R_{ii}/3$) as predicted by RDT applied to homogeneous shear flow. $R_{11}$, $R_{22}$, $R_{33}$, $R_{12}$.

where $k'^2 = k_1'^2 + k_2'^2 + k_3'^2$ and

$$
C_1 = \frac{k_3'^2}{k_1' k_3'} \tan^{-1} \left[ \frac{S\tau k_1' \sqrt{k_1'^2 + k_3'^2}}{k'^2 - S\tau k_1' k_2'} \right] + \frac{S\tau k_1' \left( k'^2 - 2k_2'^2 + S\tau k_1' k_2' \right)}{k'^2 - 2S\tau k_1' k_2' + (S\tau k_1')^2},
$$

$$
C_3 = \frac{k_3'^2}{k_1' k_3'} \tan^{-1} \left[ \frac{S\tau k_1' \sqrt{k_1'^2 + k_3'^2}}{k'^2 - S\tau k_1' k_2'} \right] + \frac{S\tau \left( k'^2 - 2k_2'^2 + S\tau k_1' k_2' \right)}{k'^2 - 2S\tau k_1' k_2' + (S\tau k_1')^2}.
$$

The variables $\hat{u}_i(k,0)$ denote the Fourier coefficients at $t = 0$. Equations 3.6 may be used to obtain analytical expressions for the energy spectrum tensor, $E_{ij} = \hat{u}_i \hat{u}_j^*$, where the "*" denotes the complex conjugate. Integration of $E_{ij}$ over the resolved wavenumbers yields the Reynolds stresses $R_{ij} = \hat{u}_i \hat{u}_j$.

4. Results

4.1. Dependence on initial spectrum

The analytical solution to the inviscid RDT equations is independent of the initial three-dimensional energy spectrum (Townsend 1976). However, the numerical solutions are not. This is seen as follows. Since the turbulence is assumed isotropic at $t = 0$,

$$
E_{ij}(k,0) = \frac{E(k)}{4\pi k^2} \left( \delta_{ij} - \frac{k_i k_j}{k^2} \right).
$$

The energy spectrum tensor may be integrated over wavenumber space in polar coordinates i.e. $k_1 = k \sin \phi \cos \theta$, $k_2 = k \cos \phi$, and $k_3 = k \sin \phi \sin \theta$, where $\theta$ varies from 0 to $2\pi$ and $\phi$ varies from 0 to $\pi$. Consider $E_{11}$. Equations 3.6 show that

$$
E_{11}(k,t) = \frac{k'^4}{(k_1'^2 + k_3'^2)^2} C_1 C_2 E_{22}(k,0) + E_{11}(k,0) + 2 \frac{k'^2}{k_1'^2 + k_3'^2} C_1 E_{12}(k,0)
$$

When $k_i' = k_i$, and $k_i$ is expressed in polar coordinates, it is readily seen that the only dependence on $k$ is through the term $E(k)/k^2$, which is common to all terms in the above
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equation. The spherical integration, \( R_{11} = \int_0^\infty \int_0^{2\pi} \int_0^{\pi} E_{11} \ k^2 \sin \phi \ d\phi \ d\theta \ d\phi \), reduces the integration over \( k \) to \( \int_0^\infty E(k) dk \) which by definition is twice the initial kinetic energy, \( q_0^2 \). The analytical Reynolds stresses are therefore independent of the initial \( E(k) \).

This is not the case when the RDT equations are numerically solved. Here, \( \frac{k_i'}{k} = \frac{k_i^j k_j}{k} \),

(no summation implied over repeated indices) which for the second-order central difference scheme

\[
\frac{\sin k_i \Delta}{k_i \Delta} \frac{k_i}{k}.
\]

(4.3)

Note that \( k_i'/k \) is still a function of \( k \). As a result, \( R_{ij} \) depends upon the initial three-dimensional energy spectrum even in the linear limit. This behavior can be explained in more general terms. The initial energy spectrum imposes a lengthscale \((1/k_0)\) and velocity scale \((u_0)\). The mean flow has no lengthscale for homogeneous turbulence, and since the evolution is linear, additional lengthscales are not generated when the RDT equations are solved analytically. As a result, the RDT equations are analytically independent of the initial spectrum. However, when the RDT equations are numerically solved, the numerical scheme imposes an effective lengthscale. As seen from figure 5, the modified wavenumber may be used to define an effective lengthscale as the wavelength below which the error in the modified wavenumber exceeds some threshold value. The result is a dependence on the initial energy spectrum. As the grid is progressively refined, \( k_i' \) approaches \( k_i \), the dependence on the initial spectrum weakens, and the numerical solution approaches the analytical solution.

Two initial spectra are considered in this paper, \( E(k) \sim k^{-2} \) and \( E(k) \sim (k/k_0)^4 e^{-2(k/k_0)^2} \).

The first choice of spectrum corresponds to the situation where the grid is so coarse that even the largest energy-containing motions are not resolved. Even a Fourier method would yield incorrect solutions under these conditions. When direct numerical simulation is performed in a channel, the minimal channel notion of Jimenez & Moin (1991) suggests that the essential dynamics of the near-wall region and outer region can be thought of as being independent and so resolved small scale turbulence near the wall is rapidly sheared. But when the near-wall region is severely under-resolved, outer layer motions that are larger than the near-wall region will experience near-wall shear. The \( k^{-2} \) spectrum attempts to model this situation. The second choice of spectrum corresponds to the situation where the energy-containing motions are resolved by the grid. A Fourier method would be expected to yield reasonable results under these conditions while less accurate numerical schemes would show the effects of discretization error.

Figure 6 shows the well-known (e.g. Townsend 1976, Rogers 1991) evolution of \( R_{i j} \) and \( R_{j i}/q^2 \) as predicted by the analytical RDT equations. Mean shear is seen to increasingly concentrate energy in the streamwise component of velocity. Shear also increases the turbulence length scales in the streamwise direction. Lee et al. (1990) note that streaks appear around \( St = 8 \). They quantify the appearance of streaks by computing the ratios, \( 2R_{11}/(R_{22} + R_{33}) \) and \( L_{uu}^i / L_{uu}^j \), where \( L_{uu}^i \) denotes the integral scale of the streamwise velocity component in the \( i \) direction. These ratios were computed from DNS of a plane channel at \( Re_\tau = 180 \) (Kim et al. 1987) and were found to have values exceeding 5 and 8 respectively in the regions where streaks were found. The RDT solutions to homogeneous shear attain these values for \( St > 8 \). Lee et al. (1990) therefore compare statistics at \( St = 8 \) to the near-wall region of the plane channel. In assessing the impact of numerical
Figure 7. The evolution of the Reynolds stresses (normalized by the initial value of $R_{ii}/3$) as a function of grid resolution when the RDT equations are numerically solved using (a): the second-order central difference scheme, (b): Fourier derivatives. The initial $E(k) \sim k^{-2}$.

4.2. $k^{-2}$ initial spectrum

Figures 7, and 8 show the effect of truncation error when the RDT equations are numerically solved. The initial three-dimensional energy spectrum, $E(k)$ varies as $k^{-2}$. This initial spectrum is chosen to model the physical situation in the channel simulations, where unresolved, small-scale turbulence is strained by the mean shear near the wall. The computational domain is $8\pi \times 2\pi \times 2\pi$, which corresponds to that used by Lee et al. (1990). The longer streamwise extent ensures that two-point correlations decay to zero in the streamwise direction, where length scales are considerably longer. Also, the effect of grid anisotropy is included. The RDT equations are solved using a second-order central difference scheme; i.e. $k'_{o} = \sin k_{o} \Delta / \Delta_{o}$ in equations 3.6. The finite-difference results are contrasted to those obtained using Fourier differentiation to isolate the effects of discretization error and truncation. Four different grids are considered – $16 \times 128 \times 16$, $32 \times 128 \times 32$, $16 \times 16 \times 16$, and $32 \times 32 \times 32$, respectively. The resolution of 128 in the $y$ direction is chosen to approximate the channel simulation where the near-wall normal...
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4.3. Resolved initial spectrum

Figures 9 and 10 show results from RDT computations where the initial spectrum corresponds to turbulence that is resolved on the computational grid prior to being sheared. The computational domain is $2\pi \times 2\pi \times 2\pi$ and the the initial $E(k) \sim (k/k_0)^4e^{-2(k/k_0)^2}$. Here $k_0$ is the wavenumber at which the spectrum peaks, and is chosen to be 10. Grids
Figure 9. The evolution of the Reynolds stresses (normalized by the initial value of $R_{ii}/3$) as a function of grid resolution when the RDT equations are numerically solved using (a): the second-order central difference scheme, (b): Fourier derivatives. The initial $E(k) \sim (k/k_0)^4 e^{-2(k/k_0)^2}$ where $k_0 = 10$. $R_{ii}$ is now less in magnitude than the exact solution. This behavior is in contrast to that observed when the initial spectrum was not resolved, and is a result of the finite-difference scheme representing the smallest resolved scales inaccurately. Figure 5 shows that differencing error in the finite-difference scheme is significant beyond $k\Delta \sim 1$. The peak in the initial spectrum corresponds to $k_0\Delta = k_02\pi/N$ where $N$ is the number of grid points in each direction. The $16^3$, $32^3$ and $64^3$ grids yields values of $k_0\Delta$ of 3.93 (unresolved), 1.96 and 0.98 respectively. The resulting truncation error has the effect of ignoring the energetic
scales in the initial condition, the growth in energy in those scales due to mean shear is not represented, and the net result is an underprediction of the Reynolds stresses.

### 4.4. An explanation

The similarity between the coarse channel and numerical RDT solutions for the initially unresolved spectrum suggests that the RDT equations may be used to provide an explanation for the behavior in the channel. Consider the momentum equations in 3.4. The only variable being spatially differentiated is the fluctuating pressure. Truncation error would therefore entirely result from errors in approximating the spatial derivatives in pressure, and then projecting the velocity field to ensure the divergence–free condition. Note that this error includes the effects of both excluding high wavenumber modes, and discretization error in differentiating the resolved modes. The analytical derivatives are exact for the resolved wavenumbers, but exclusion of high wavenumber information implies that the derivatives in physical space are incorrect. Using finite–difference or finite–volume schemes to compute the spatial derivatives increases the error since even the resolved wavenumbers are not differentiated exactly.

It can be argued that the error in pressure derivatives will also dominate the chan-
nel simulations. Truncation error increases as the order of the spatial derivatives being computed increases. The highest derivatives in the channel are the second derivatives in the Laplacian operator which appears in the viscous term, and pressure Poisson equation. Section 2 shows that errors in the channel simulations are insensitive to Reynolds number. This suggests that the pressure equation is the larger contributor to truncation error.

The evolution equations for the Reynolds stresses in the RDT limit allow further clarification. We have

$$\frac{d}{dt} R_{11} = -SR_{12} - u_1 \frac{\partial p'}{\partial k_3},$$

$$\frac{d}{dt} R_{22} = -u_2 \frac{\partial p'}{\partial k_2} + St \ u_2 \frac{\partial p'}{\partial k_1} + St \ u_2 \frac{\partial p'}{\partial k_1},$$

and

$$\frac{d}{dt} R_{33} = -u_3 \frac{\partial p'}{\partial k_3}.$$

The Reynolds shear stress, $R_{12}$ combines with mean shear to ‘produce’ $R_{11}$. The pressure–strain correlation, $u_1 \frac{\partial p'}{\partial k_3}$ acts to redistribute energy from $R_{11}$ to the other two components. Both the coarse channel, and RDT results, show that $R_{11}$ is higher than expected, although $R_{12}$ is smaller or even equal to the correct value. In other words, $R_{11}$ is higher although the production term is smaller. This is only possible if the pressure–strain correlation is not large enough. Figure 11 shows the pressure-strain correlation in the $R_{11}$ equation in the RDT limit. The pressure–strain term is indeed smaller at coarse resolutions for all resolutions considered.

Suppression of the transfer from $u_1'$ to the other components may be considered a result of constraining the velocity field to be divergence-free in the presence of truncation error. Pressure acts to satisfy $\frac{\partial u_1'}{\partial x_1} = 0$, which in Fourier space implies

$$k_1 \tilde{u}_1 + \left( k_2 - St k_1 \right) \tilde{u}_2 + k_3 \tilde{u}_3 = 0;$$

(4.6)

i.e., the Fourier coefficient of the velocity vector is perpendicular to the wavenumber
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vector, \( \mathbf{k} = k_1 e_1 + k_2 e_2 + k_3 e_3 \). When continuity is imposed numerically, the velocity vector is now constrained to be normal to the modified wave-number vector \( i.e., 
\[
k'_0 \mathbf{u} + (k'_2 - S t k'_1) \mathbf{u} + k'_3 \mathbf{u} = 0.
\]

First, consider the impact of ignoring high wave-number information. The resolved modes are differentiated exactly and the velocity vector lies in the plane normal to the wave-number vector. As done by Rogallo (1981), define an orthogonal basis, \( e'_1, e'_2, e'_3 \), such that \( e'_3 \) is parallel to the wavenumber vector. \( e'_1 \) and \( e'_2 \) therefore lie in the plane perpendicular to the wavenumber vector. The velocity vector may therefore be expressed as:
\[
\mathbf{u}'(k) = \alpha(k) e'_1 + \beta(k) e'_2.
\]

Here, \( \alpha \) and \( \beta \) are complex, and depend only on the magnitude of the wavenumber vector, \( k \). The basis \( e'_1, e'_2, e'_3 \) is arbitrary, subject only to the constraint that \( k e'_3 = k \). Assuming that \( e'_1 \cdot e'_3 = 0 \) (\( e'_3 \) denotes the unit vector in the \( x_3 \)-direction) yields a solution for \( e'_2 \) and \( e'_3 \), which in turn yields the following expression (Rogallo 1981) for the velocity vector in Fourier space:
\[
\tilde{u}_1 = \frac{\alpha k_2 k_3 + \beta k_1 k_3}{k \sqrt{k_1^2 + k_2^2}}, \quad \tilde{u}_2 = \frac{\beta k_2 k_3 - \alpha k k_1}{k \sqrt{k_1^2 + k_2^2}}, \quad \tilde{u}_3 = -\frac{\beta \sqrt{k_1^2 + k_2^2}}{k}.
\]

Equation 4.9 shows that the relative values of the velocity components change if their projections in the plane perpendicular to the wavenumber vector (\( \alpha \) and \( \beta \)) change. It can be shown that ignoring high-wavenumber modes changes \( \alpha \) and \( \beta \). Equation 4.8 shows that \( \alpha \) and \( \beta \) are subject to the constraint (Rogallo 1981),
\[
E(k) = \int (\alpha \alpha^* + \beta \beta^*) dA(k)
\]

where \( E(k) \) denotes the three-dimensional energy spectrum, the brackets \( <> \) denote the expected value, and the superscript, * denotes the complex conjugate.

Note that the integration is performed over a spherical shell in wavenumber space. However, a discrete grid on a rectangular domain does not represent a spherical shell in Fourier space. This distinction becomes increasingly important when the rectangular domain is anisotropic, or the grid resolution is coarse. Representing the velocity field on a coarse grid on a rectangular domain is therefore equivalent to filtering the three-dimensional spectrum. This implies (equation 4.10) that \( \alpha \) and \( \beta \) differ from their values in the absence of such filtering, which (equation 4.9) changes the individual velocity components. Discretization error compounds the error, since the velocity components are now constrained to be normal to the modified wave-number vector (equation 4.7). The basis vectors, \( e'_i \) in equations 4.8 and 4.9, are now defined in terms of the modified wavenumber. As a result, the wavenumbers in the expression for the velocity components after satisfying continuity (equation 4.9) are replaced by the modified wavenumbers. Thus, discretely satisfying continuity on a coarse grid changes the relative values of the velocity components.

5. Summary

This paper uses rapid distortion theory to study the truncation error in boundary layer simulations at coarse resolution. The study is motivated by the fact that large-eddy simulations of attached boundary layers at high Reynolds numbers require very fine
near–wall resolution when the LES equations are integrated down to the wall. The paper considers the question of whether common subgrid models are modeling the dominant physical/numerical effect of the subgrid scales in the inner–layer region. Most subgrid models are required to model the net nonlinear transfer of energy from the resolved scales to the subgrid scales. However, Kline et al. (1967), Uzkan & Reynolds (1967), and Lee et al. (1990) suggest that streaks, which dominate the near–wall region, are produced by the linear mechanism of rapid straining of turbulent fluctuations. Lee et al. (1990) in particular, establish a close connection between turbulence in the viscous sub–layer, and homogeneous turbulence that is sheared at very high shear–rates. They also show that the evolution of rapidly sheared homogeneous turbulence is well described by linear RDT and that the RDT can reasonably predict the Reynolds stress anisotropy and structural features of near–wall turbulence.

This paper therefore considers the possibility that the errors involved when numerically solving the RDT equations on a coarse mesh might correspond to the errors in the near–wall region on coarse meshes. The discretized RTD equations, thus obtained, can be solved analytically using the notion of ‘modified wave–number’. This solution which is a straightforward extension of the classical analytical solutions of Townsend (1976) represents the effects of both, filtering and discretization error associated with the spatial differencing scheme. Two cases are considered, one where the mesh is so coarse that the energy–containing motions are not resolved, and the second, where the energy–containing motions are resolved, but the smaller scales suffer from discretization error. Even Fourier discretization will yield inaccurate results in the first case, while the second case is one where Fourier discretization yields reasonable results but finite difference discretization does not.

The numerical RDT results for the case where even the large–scales are not resolved show similar trends to channel flow simulations on coarse grids; i.e. at coarse resolutions, the streamwise component of kinetic energy is higher, while the vertical and spanwise components are lower than their exact values. The RDT equations are used to suggest that the dominant source of error arises from the discrete Poisson equation for pressure since pressure is the only variable being differentiated in the linear homogeneous limit. Both truncation and discretization error yield inaccurate representations for the Laplacian operator in the pressure equation. Inversion of the Laplacian operator yields inaccurate pressure fields which in turn yields inaccurate velocity fields. An equivalent interpretation is that the pressure field is obtained by constraining the velocity field to be divergence–free. However, each of the individual derivatives, $\partial u_i / \partial x_j$, is incorrect due to truncation and discretization. The sum of the three gradients is still constrained to be zero. In terms of the Reynolds stresses, this error shows up in the pressure–strain correlation. Truncation error appears to suppress the transfer of energy from the streamwise component of velocity to the vertical and spanwise components, yielding higher values of the streamwise component, and lower values of the vertical and spanwise components.

This suggests that, near the wall, it is probably more important to account for the effect of the subgrid scales on the non–local effects of pressure than it is to model their nonlinear effects due to advection. One way to achieve this might be to use the equivalent of Reynolds stress modeling for LES, where the pressure–strain correlation would be explicitly modeled. Another possibility is to retain presently used models for the subgrid stress, but allow the velocity field to have a finite–divergence. This divergence could be modeled in a variety of ways. e.g. $\sim C \Delta_j \partial u_i / \partial x_j$ where $C$ is a constant that could be obtained from DNS data, or obtained dynamically similar to Germano (1991), and $\Delta_j$.
Rapid distortion theory applied to under-resolved boundary layer simulations denotes the filter width in each coordinate direction, which ensures that the velocity field is divergence-free in the DNS limit.

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